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CALCULATION OF SURFACE BINDING ENERGIES BY COMPUTER SIMULATION OF THE SPUTTERING PROCESS

JOHN PALMER JOHNSON

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CALCULATION OF SURFACE BINDING ENERGIES BY COMPUTER SIMULATION OF THE SPUTTERING PROCESS

by

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ABSTRACT

Sputtering of monocrystalline copper, a face-centered cubic, was investigated by computer simulation techniques using the Born-Mayer potential. Normally incident argon ions were shot into the (111), (110), and (100) orientations at various energies. Qualitatively correct deposit patterns were obtained for all orientations. Surface irregularities were found to play a significant role in the sputtering mechanism. Approximate values for the surface atom binding energy on the (111) and (110) orientations were 2.25 eV and 3.0 eV, respectively.

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1. Introduction.

Cathode sputtering, the emission of particles from a material when bombarded by ions or atoms, is hardly a new topic. This phenomenon was first observed by Grove [1] in 1852. In the following years sputtering introduced problems in the design and construction of electron vacuum tubes. More recently, interest has been revived in sputtering because of its importance in the development of the ion engines, fusion reactors, and space vehicles.

Kingdon and Langmuir proposed the first theoretical model of the sputtering mechanism in 1923 [2]. The "momentum transfer" mechanism described in this paper breaks the sputtering process down into two stages. In the first phase, the primary ions are presumed to strike surface atoms of the crystal, driving them into the crystal, and forming depressions on the surface. In the second phase, succeeding primary ions impact at the bottom of these depressions. With the presence of these depressions the primaries interact deeper in the crystal and, therefore, with stronger force fields. As a result, the time required to complete the interaction is less, and, correspondingly, energy losses are reduced. It is concluded that such interactions as these in the second phase can be considered elastic and that the primary may retain a significant portion of its initial energy. These atoms then may strip out atoms from around the edge of the depression as they recoil.

Blechschmidt and von Hippel [3] and, later, Townes [4] proposed an evaporation model based on heat transfer laws. This theory was predicated on the idea that incident particles heated a limited volume of the target material to a rather high temperature and, as this heat was dissipated, surface atoms

were ejected by evaporation.

In 1948 Bohr [5]demonstrated that radiation damage in the sputtering energy range could be treated classically.

Next, Keywell [6]suggested an explanation of sputtering based on the theory of neutron diffusion. He restricted his arguments to primary energies less than six KeV and presumed a succession of "hard-sphere", random collisions. Using some of Keywell's data, Harrison [7, 8]was able to fit a statistically derived expression involving four parameters (one of which was known initially and another became known later [9]) to the sputtering ratio-primary energy curve. Neither of these theories included the regularities of the crystal geometry.

Henschke [10]and Lanberg [11]offered analytic solutions to the low-energy cathode sputtering problem based on the binary collision process described in the following paragraph. On the differences between the two models, Lanberg says,

> ...Henschke [10]assumes that the ejecting collision is always between the deflected ion and an atom; the analysis presented here postulates a final collision between two lattice atoms. The former work [10]uses a rigid collision radius and the theory of collisions with restitution; here, a Morse curve collision interaction is presumed, and from it, both energy transfer and loss to the lattice is found. ...this analysis arrives at the experimental threshold values without the use of adjustable constants. [11]

while such constants are required by Henschke. Both works use the momentum transfer ideas of Kingdon and Langmuir.

Recently, work has been done by Gibson, Goland, Milgram and Vineyard [12], Robinson and Oen [13, 14, 15], Erginsoy, Vineyard, and Englert [16], Harrison and Gay [17], and Levy [18]and others towards simulating the radiation damage mechanism in digital computers. So far two general approaches

have been used; a many-bodied collision process and a binary collision process. The binary process, as its name implies, involves a two-body interaction, while the many-bodied approach integrates numerically the force laws operating between a given atom and a number of other atoms. Gay and Harrison [17] showed that for target points within a certain impact parameter of the target atom these two processes result in similar energy transfer, but outside this region binary collisions transferred less energy than the many-bodied process. They also demonstrated that for large impact parameters the primary scattering angle was reduced and the recoil angle was increased when the binary process was applied.

2. The Model.

This project uses the Gay-Harrison model [16] as modified by Levy [18]. Certain further modifications have been incorporated and will be outlined later.

In general, the Gay-Harrison model assumes all collisions to be n-bodied. In this process, the primary (bombarding ion), through collisions, displaces atoms of the target crystal. These atoms in turn experience further collisions with other atoms of the crystal. Eventually, some atoms become directed toward the bombarded surface and are ejected, or cause other atoms to be ejected, provided they have sufficient kinetic energy to overcome the forces operating at the crystal surface.

The choice of potential is the Born-Mayer. Gibson, Goland, Milgram and Vineyard [12] found that this potential should be satisfactory for collisions below seven KeV. This potential can be written in the form, $V(r) = \exp(A+Br)$, where "B" is always negative and "r" is the separation distance of the interacting particles. This function is modified to an eroded form so that the potential and the force go to zero at a distance equal to the nearest-neighbor-distance of the crystal. This makes the micro-crystallite stable prior to the impact of the primary and, hence, the total energy of the system at all times is the initial kinetic energy of the impacting primary.

The erosion of the potential is performed as soon as any particle comes within a sphere of radius ROE (ROE is the nearest-neighbor-distance) about any other particle. At the end of this time step the potential is calculated according to $V = V(r)-V(ROE)$ where "r" is the separation distance of the interacting particles. It is the assumed that one-half of this "pair-wise" potential energy, V, is associated with each of the interacting particles.

Therefore, the "pair-wise" potential is equal to zero at r = ROE but has a non-zero value at any other location where the separation distance is less than the nearest-neighbor-distance.

The forces are eroded in a similar fashion. If two particles are farther apart than ROEM (a distance less than ROE by one time step) but nearer than ROE, the force is found from F = F(r) - V(ROE)/DTI, where DTI is the basic time step interval. However, if the particles are separated by less than ROEM then the force is merely F = F(r). See Figure 1 for a graphical portrayal of the force-potential erosion process.

The forces derived from the potential are handled by a double iteration technique. Newton's Law, F = ma, can be expressed, $F(\Delta t/m) = \Delta v$, and the change in position related to the change in velocity by, $RX_{I+1} = RX_I + (VX_I + \Delta VX/2)\,\Delta t$, where an average velocity during movement is assumed. The force from which ΔVX is calculated is found as follows:

(a) Assume an atom at an initial location and calculate the sum of all forces acting on it (resulting from all atoms within a radius of one "nearest-neighbor-distance").

(b) Move the atom to the location resulting from application of this force and calculate the resultant force operating on the particle in this new location in the same fashion.

(c) Move the atom back to its original location and move it from there according to the average of the forces resulting in steps (a) and (b).

Thus, the atom has been moved to its new location. This process applied to all atoms constitutes one time step. The fact that some atoms are excluded from this process will be discussed later. A "time step multiplier" is included in the computer program so that these calculations may be made as

frequently as desired.

Investigation showed that the sputtering ratio (defined as the number of atoms from the crystal ejected through the bombarded surface per incident primary) could be maximized with respect to the "A" potential parameter and minimized with respect to the "B" potential parameter. The extrema were in the range A = 12 to A = 13, and B = -7.6 (approximately). Using experimental data of Carlston and Magnuson [19], Harrison [20] calculated values for the parameters of the Born-Mayer potential for the copper-copper and argon-copper interactions and showed that the "A" parameter should be 11.435 for argon-copper in the center of mass system. Correcting this to the laboratory system, $E_{cm} = \frac{1}{2}(m_b + m_t)[v_b m_b/(m_t + m_b)] = E_o[m_b/(m_t + m_b)]$, where m_b and m_t are the bullet and target masses respectively, v_b is the bullet initial velocity, E_{cm} is the energy of the center of mass, and E_o is the total energy of the system in the laboratory frame. Now, the energy of the particles in the center of mass is equal to $E_o - E_{cm} = E_o[m_t/(m_t + m_b)]$. Evaluating this for the argon-copper system and applying the correction to the potential expression, the "A" parameter becomes 11.923. A slightly different value was used in this investigation, However, the plot of "A" versus the sputtering ratio shows that the sputtering ratio is relatively insensitive to variations in "A" so long as a choice is made in the vicinity of the extremum. Because of this argument and the success of Levy and Harrison [18] with nearly these same values, the following choice of parameters was made.

System	A	B(lattice units)$^{-1}$
A-Cu	12.560	-7.597
Cu-Cu	10.024	-9.197

Each of the three orientations under investigation, (111), (110), and (100), has been examined for inherent symmetries and, based on these, representative target areas have been selected. Furthermore, a number of target points were chosen within each representative area. See Figures 2, 3, 4, and 5.

Other major features of the model are as follows.

(a) Thermal motion of the atoms of the microcrystallite has been neglected.

(b) Interactions of the electrons of the microcrystallite and all other bodies have been disregarded.

(c) Cohesive and restoring forces do not appear in the computer program but have been taken into consideration in the calculation of the sputtering ratios and the deposit pattern investigation.

3. The Program

a. TWOPOT

The model is simulated on a CDC 1604 computer. The program is written in FORTRAN 60 and FORTRAN SYMBOLIC. Basically, the program constructs the copper microcrystallite, injects a primary argon atom at a specified point and with a specified energy, calculates the movement of the primary and the atoms of the microcrystallite through a series of time steps, and shuts down after a specified number of time steps or when the total potential energy of the system becomes less than 0.5 electron volts. This program gives a system energy total that remains within 3.5% of the initial primary energy at all times.

During the investigation of the effect of surface irregularities on (111) sputtering two nearly identical programs were used to simulate a left and right microcrystallite. This became necessary when it was found that an inordinate amount of energy was being lost by atoms escaping through the "sides" of the crystal. These two crystals were designed to have an overlap so that values resulting from one could be checked against the other. The composite crystal contained 210 atoms.

The program contains a variable, LCUT, LCUT is defined as zero for any atom with potential energy greater than some arbitrary quantity and one otherwise. This quantity, LCUT, serves two purposes. One, it results in a saving of computer time since those atoms with LCUT = 1 are not considered in force calculations. Two, it facilitates the introduction of surface irregularities into the crystal. For example, a depression can be produced by setting LCUT of a surface atom equal to one initially. Under this condition the atom is effectively removed. Other modifications of the surface geometry are

possible with combinations of atoms removed in this fashion.

Further irregularities can be introduced on the crystal surface by inserting the desired initial coordinates of atoms to be added to the crystal. This must be done carefully to insure the atom(s) are placed in a potential-free position. Otherwise, the crystal is not initially stable.

An index, KCUT, has been introduced to show which of the original crystal boundaries a sputtered atom passed through. KCUT for all atoms is zero at the start of the run. At the end of each time step the coordinates of all atoms with KCUT = 0 (still inside the crystal) are tested against the original physical limits of the crystal. If an atom is outside any of these crystal bounds, KCUT is given a value from one to six indicating which boundary it has exceeded and is excluded from further testing. This was inserted to facilitate the analysis of those cases where an atom's coordinates indicated it was sputtered but where there was doubt about which crystal surface the departing atom passed through.

The program provides a summary of sputtered atoms at the end of each run. It should be mentioned that this summary includes those atoms that are still within the confines of the crystal but whose velocity is in the proper direction and whose energy is great enough that they merit special consideration. The final disposition of such atoms is primarily a matter of judgment.

b. SPOTA

This auxiliary program was written to provide as the output a stereographic plot of the angular distribution of the sputtered atoms. The input is in the form of the velocity components of the atoms found to have been sputtered in TWOPOT. Essentially,

the program calculates the kinetic energy in the direction perpendicular to the bombarded surface and subtracts a quantity appropriate to the energy loss an atom would experience in overcoming the binding forces at the crystal surface. The new "perpendicular velocity" component is found and the ratios of the other two components to this one are calculated. A subroutine, DRAW, is called to plot these two ratios, one against the other.

Because of the six-way symmetry of the representative area of the (111) orientation, there are five more points corresponding to each of those calculated as in the above paragraph. Each of these five results from a rotation of the original. Program SPOTA calculates and plots these rotations also.

4. Results and Discussion

A. Parameter Investigation

The (111) orientation was chosen for this investigation and bombarded with a ten KeV primary. Runs were then made with various combinations of the potential parameters, "A" and "B". The sputtering ratio was plotted as a function of each parameter for selected values of the binding energy, with results shown in Figures 6 and 7.

We see that the sputtering ratio can be maximized with respect to the "A" parameter and minimized with respect to the "B" parameter. (It is not known whether these are relative or absolute extrema.) Furthermore, both these extrema occur very near the semi-empirical values of Harrison, Carlston and Magnuson [20], based on the experiments of Carlston, Magnuson, Mahadevan and Harrison [21]. These values of "A" and "B" then designate a saddle point on the surface formed by plotting the sputtering ratio against these two parameters, but we do not know why this condition results.

These plots illustrate another interesting point: the sputtering ratio varies slowly with parameter variation near the extrema. Hence, the model results should be independent of detailed knowledge of the exact values for these parameters.

B. Deposit Patterns

Computer runs were made on all three orientations, (111), (110), and (100) with the potential parameters indicated earlier. Then a plot was made of the ratio of the x-velocity to the y-velocity versus the ratio of the z-velocity to the y-velocity. These points were rotated and reflected as required to include the various possible orientations of the basic representative area. These transformations follow directly from symmetry considerations.

Physically, these plots are equivalent to an experiment in which a plane collector is placed parallel to the bombarded surface and a unit distance from it. Figures 8, 9, and 10 show, respectively, the trigonal symmetry of the (111) orientation and the four-way symmetry of the (100) and (110) orientations.

The dependence of the deposit patterns was examined in runs where the Gibson 2 parameters were used for the argon-copper interaction as well as the copper-copper. Figure 11 shows the result on the (111) orientation at a primary energy of three KeV.

Examination of Figures 8, 9, and 10 show that the Gay-Harrison computer simulation model is yielding qualitatively correct deposit patterns. These patterns are meant to illustrate only that the proper shape of the spot patterns is being achieved. Binding energies are not shown since the (110) and (100) orientations have not been investigated in detail. These patterns are to be compared with those of Andersen and Wehner [22] and Southern, Willis and Robinson [23].

The (111) orientation (see Figure 8) exhibits a diffuse central spot and three other spots. The (100) orientation (see Figure 9) shows the beginnings of four ⟨011⟩ spots and a central spot. Both of these agree qualitatively with the experimentally observed patterns. The (110) orientation (see Figure 10) has two ⟨001⟩ spots and a central ⟨110⟩ spot but there are no experimental patterns with which to compare this.

As is discussed in the next section, it should be kept in mind that the location of these spots is sensitive to the choice of surface binding energy and they can be moved about within a range by adopting different binding energy values.

For many years these spots in the deposit patterns have

been believed to be evidence supporting the momentum focusing ideas of Silsbee [24]. Silsbee argued that preferential sputtering should occur in the close-packed directions of the crystal because of this momentum focusing.

The significance of the deposit patterns resulting from the computer simulation lies in the fact that we [18, 25] found, using this identical computer model, that Silsbee chains were not contributing significantly to the sputtering process. We did not deny the existence of such focusons but did not need their contribution to produce results commensurate with experimental data. We found that even at 10 KeV practically the entire sputtering event is contained in the first four layers of the crystal. Therefore, any directional preference must be attributed to glancing collisions at the crystal surface.

C. Effect of Surface Irregularities

This investigation was designed to determine the effect of imperfect crystal surfaces on the sputtering process. To do this, various surface irregularities were introduced into the crystal. Atoms were removed from the crystal surface by setting the LCUT parameter equal to one to remove the desired atom. Additional atoms were added to the surface by reserving an atom index for the added atom and inserting the atom's initial coordinates (RX, RY, RZ) in terms of the crystal geometry parameters, SCX, SCY, and SCZ. These atoms must be positioned so that there was initially no interaction between the added atom and the basic crystal. Otherwise, an additional amount of energy (other than that of the primary) appears in the system.

In this investigation an inordinate number of high and moderate energy atoms were lost out the crystal boundaries in the x-direction. Consequently, two crystals of the size of

Levy's [18] were used side by side and with an overlap so that a check could be made on the duplicated atoms.

These crystals were run with various combinations of running time and time step interval to determine the combination with which the sputtered atoms could be discerned but with a minimum of computer time. All runs were terminated when the total potential energy of the system was less than one-half eV. However, the time step intervals were varied depending on the type of surface irregularity involved and the proximity of the target point to this irregularity.

Plots were made of the sputtering ratio versus surface binding energy for the cases of (1) regular surface, (2) an atom removed from the surface within the representative area, and (3) an atom added to the surface within the representative area. These were accomplished for the (111) orientation with a seven KeV primary and for the (110) orientation with a three KeV primary. These plots are shown in Figures 12 and 13.

Deposit patterns were made for the "regular", "hole", and "stub" crystals for the (111) orientation at seven KeV to examine any variations with surface irregularities. These are shown in Figures 14, 15, and 16. Figure 21 shows a composite spot pattern that was made assuming equal proportions of "regular", "hole", and "stub" type surfaces. All these patterns were drawn with a scale of one-half unit per inch. The binding energies in these figures are 2.0, 2.5 and 4.0 eV. In Figure 21 the binding energy is 2.0 2.25 eV.

Ejection patterns as a function of surface binding energy were also made for the (111) orientation with the "hole" crystal. These results are shown in Figures 17, 18, 19 and 20.

Examination of Figures 12 and 13 demonstrates that the presence of irregularities in the crystal surface have a definite effect on the sputtering ratio. Only the (111) orientation at seven KeV and the (110) orientation at three KeV have been examined in detail. However, it is reasonable to presume that these orientations at other primary energies will yield similar results.

These plots together with some of the deposit patterns should greatly facilitate a determination of the surface binding energy. Levy first attempted to build a binding energy into the basic program as a variable quantity. This necessitated a complete run for each new value of the binding energy and was prohibitive in computer time. His solution was to take any atom moving away from the microcrystallite as a sputtered atom. This was later modified to consider only those atoms with negative y-velocity. Sputtering ratio curves can be drawn by eliminating those atoms in this set which do not have enough energy to overcome a specific value of surface binding energy. It is obvious that an approximate value for this binding energy would be invaluable as a starting point for other surface physics investigations. To that end, the surface binding energy can be limited to a range by curves such as Figures 12 and 13, and can be specified even further by adjustment of the spot patterns as in Figures 17, 18, 19, and 20.

As can be seen in the (111) data, both the types of irregularities tested thus far have produced much higher sputtering ratios for a given value of the surface binding energy than was obtained from the regular crystal surface; the "hole" producing much the greater effect especially at low values of the binding energy. To achieve the Magnuson-Carlston [26] experimental value of 9.6 for the sputtering ratio, the "regular" model required

a surface binding energy of 0.5 eV where the "stub" model required the more realistic figure of 2.3 eV and the "hole" required 4.2 eV. It might, with some assurance, then, be stated that the (111) surface binding energy lies between 0.5 and 4.2 eV.

Similar results were obtained for the (110) orientation at three KeV. The big difference, however, lies in the magnitude of the effect. Surface irregularities seem to have much less influence on the (110) surface. Again, the magnitude of the effects follows the same pattern as on the (111) surface, that is, the "hole" model produces the greatest sputtering ratio, the "regular" model the least, and the "stub" falls in between. By analysis similar to that for the (111) surface, it appears that the surface binding energy on the (110) surface lies between 2.6 and 5.7 eV. The difference in the magnitude of the effect of irregularities on the (111) and (110) orientations explains why Levy [18] was able to get a good fit to the Magnuson-Carlston (110) data but not their (111) data.

Figures 14, 15, and 16, depicting deposit patterns for the "regular", "hole", and "stub" models in the (111) orientation, all show the characteristic trigonal symmetry. The best patterns occurred at different binding energy values but this was to be expected. The spots also occur at slightly different positions. Figures 17, 18, 19, and 20 demonstrate that the spots move and change in quality depending on the value of the surface binding energy and eventually become so diffuse as to be unrecognizable when the binding energy reaches unrealistically high values. Figure 21 shows a composite spot pattern where all three types of surface have been given equal weight. This pattern looked most like the experimentally observed pattern at a binding energy of 2.25 eV. This value falls in the range we would expect from

Figure 12 and may be taken as a starting point for further investigation of the (111) orientation.

Similar analysis led to a value of 3.0 eV for the binding energy of the (110) surface. This is also in the expected range (see Figure 13) and should be a good first approximation to the actual binding energy for that orientation.

Our latest investigations show the surface binding energy on the (111) orientation with a 3 KeV primary to be 0.5 eV to 3.6 eV. This compares favorably with the results from the 7 KeV primary and, therefore, reinforces the above argument. Our latest observations have also uncovered the possibility that a reasonable approximation to real (111) surface conditions may be obtained from the "stub" model. The sputtering ratio vs. binding energy curve for this configuration seems to fall between that of the "hole" and "regular" models. Furthermore, it seems to provide the Magnuson-Carlston sputtering ratio at approximately the proper binding energy.

The real test of this model requires some distribution of "stub", "hole", and "regular" models that will yield the experimentally observed deposit patterns and weighted sputtering ratio curves that will fit the Magnuson-Carlston data at all energies. Furthermore, both these objectives will have to be accomplished with the same surface binding energy value on a given surface for all primary energies. Even without knowledge of the factors influencing the above-mentioned distribution, the dependence upon surface irregularities is so great that any attempt at an analytic solution to the sputtering problem is probably futile.

5. Summary

Five significant things have come out of this study. First, it was found that the potential parameters necessary for reasonable results specify a saddle point in the plot of the sputtering ratio versus the two parameters. This is intuitively satisfying but remains unexplained physically.

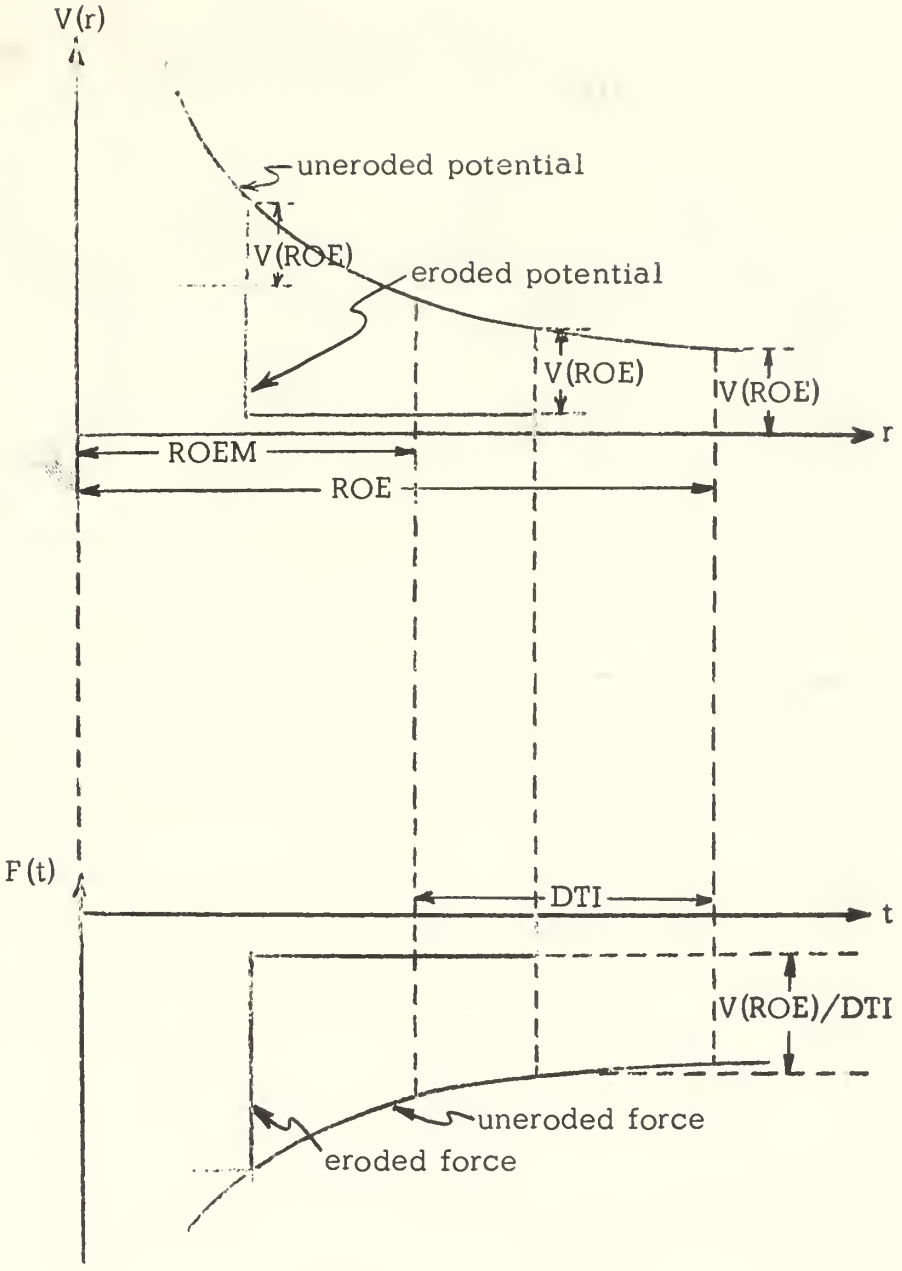
Second, it appears that surface irregularities play such a significant role in the sputtering process that analytic approaches to the sputtering problem may be prohibitively difficult.

Third, reasonable agreement with experiment can be achieved without reliance upon the Silsbee focusing mechanism.

Fourth, it appears that real (111) orientation surface conditions may be approximated by the "stub" model. This would greatly reduce the computer time now necessary to accomplish a complete run. This hypothesis needs further investigation to insure its validity on the (111) orientation and to determine if it can be extended to other orientations.

Fifth, and most important, the analysis of deposit patterns provides an excellent first approximation to the surface binding energy. Hopefully, this, in conjunction with the sputtering ratio versus binding energy plots, will yield sputtering ratio curves that compare favorably with those experimentally observed for all orientations and primary energies, thereby providing a greater insight into the sputtering mechanism.

The assistance of all personnel associated with the computer facility is gratefully acknowledged. The guidance and assistance of Professor Don E. Harrison, Jr., in all facets of this work was invaluable.



Computer Simulation
Force-Potential Erosion Process
Figure 1

Face Centered Cubic (111)

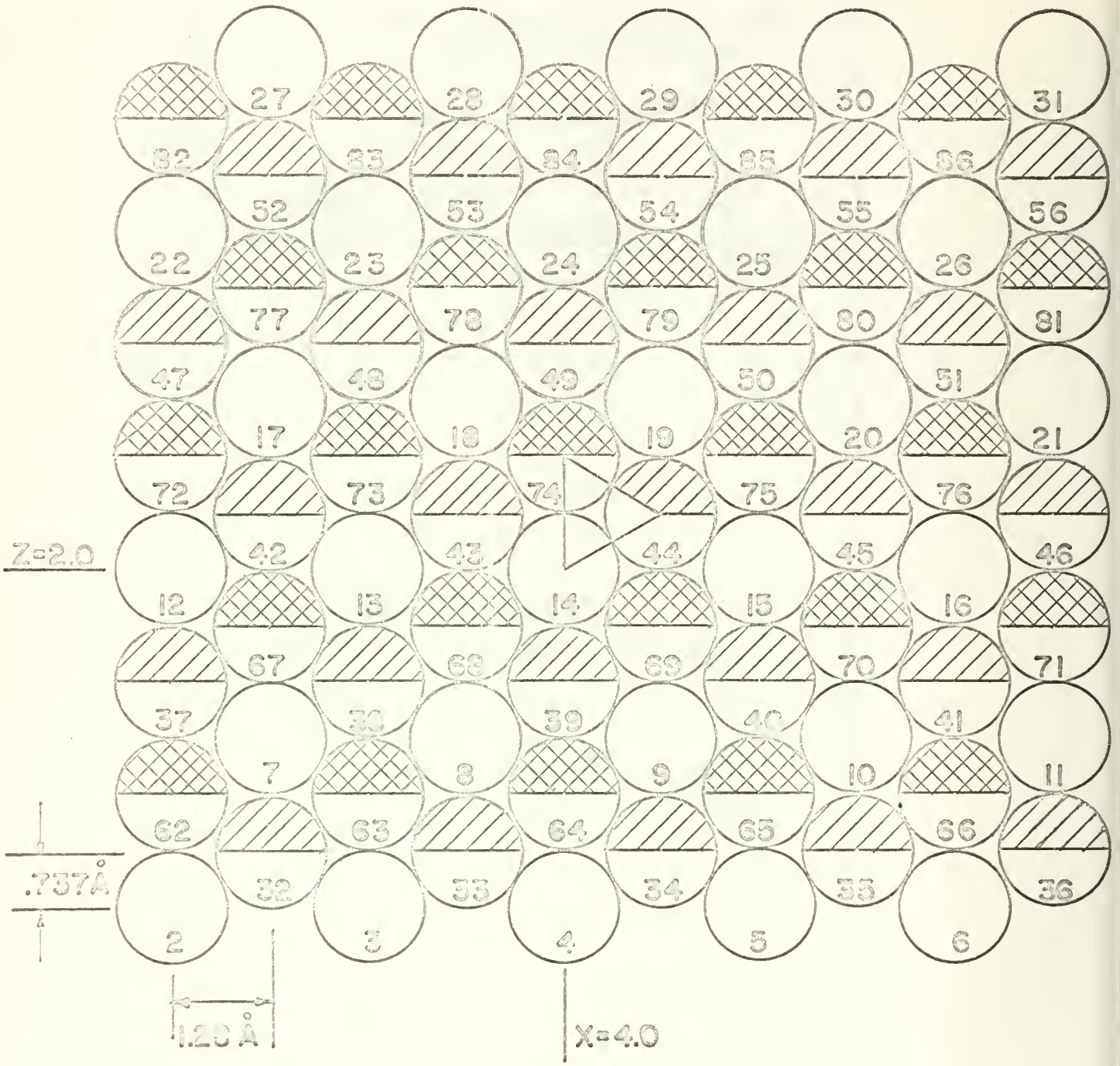


Figure 2

FACE CENTERED CUBIC (110)

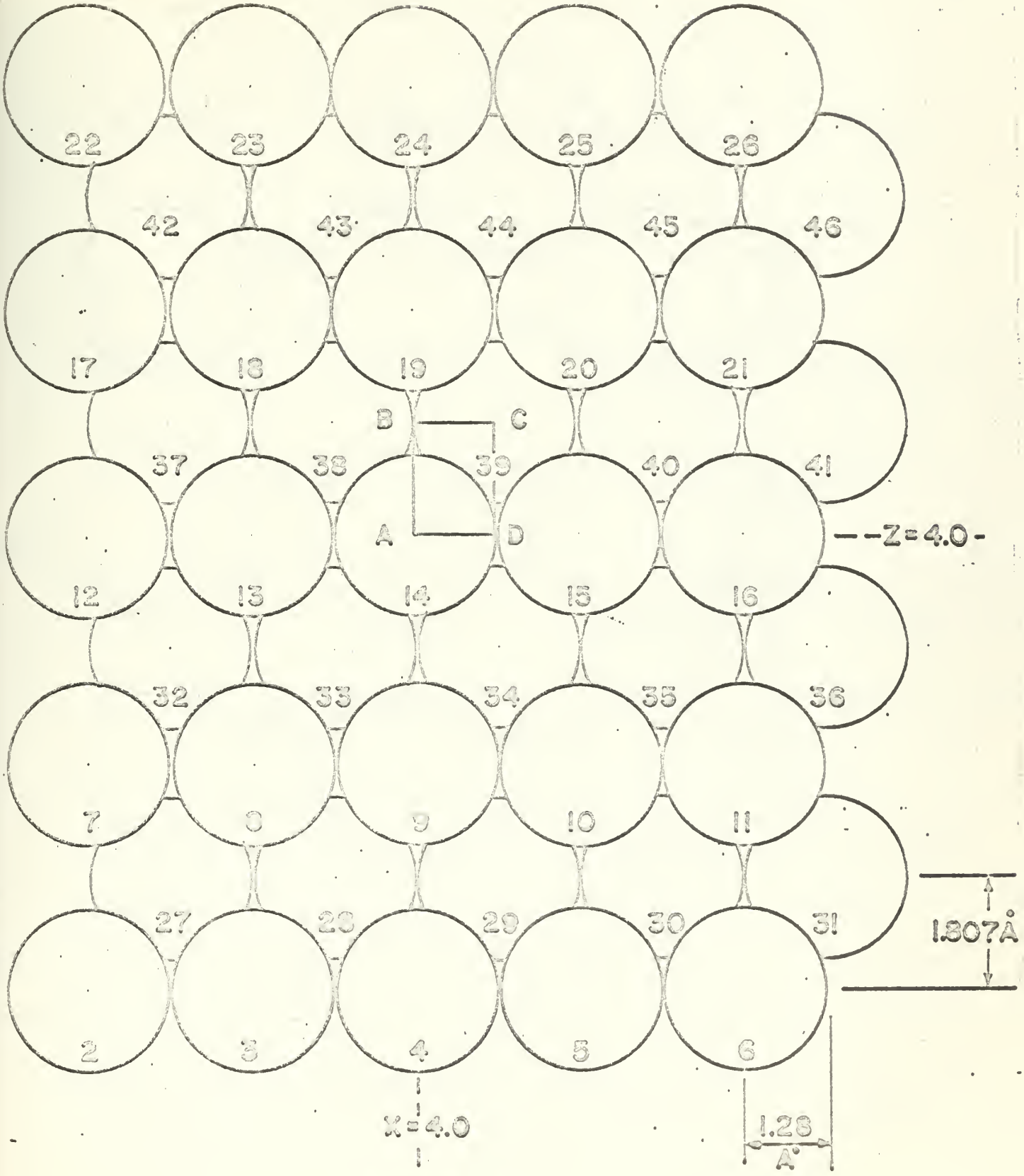


Figure 3

FACE CENTERED CUBIC (100)

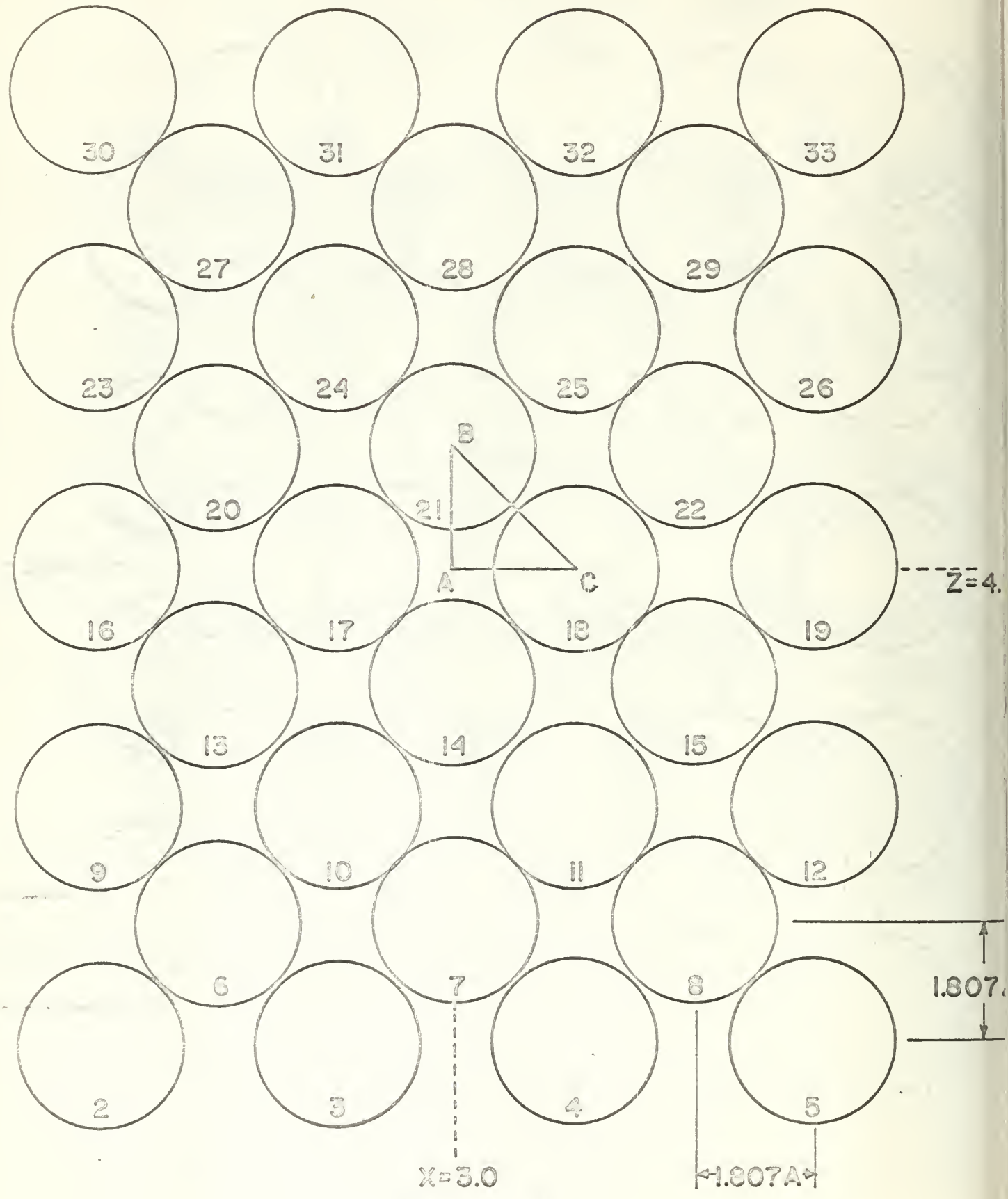


Figure 4

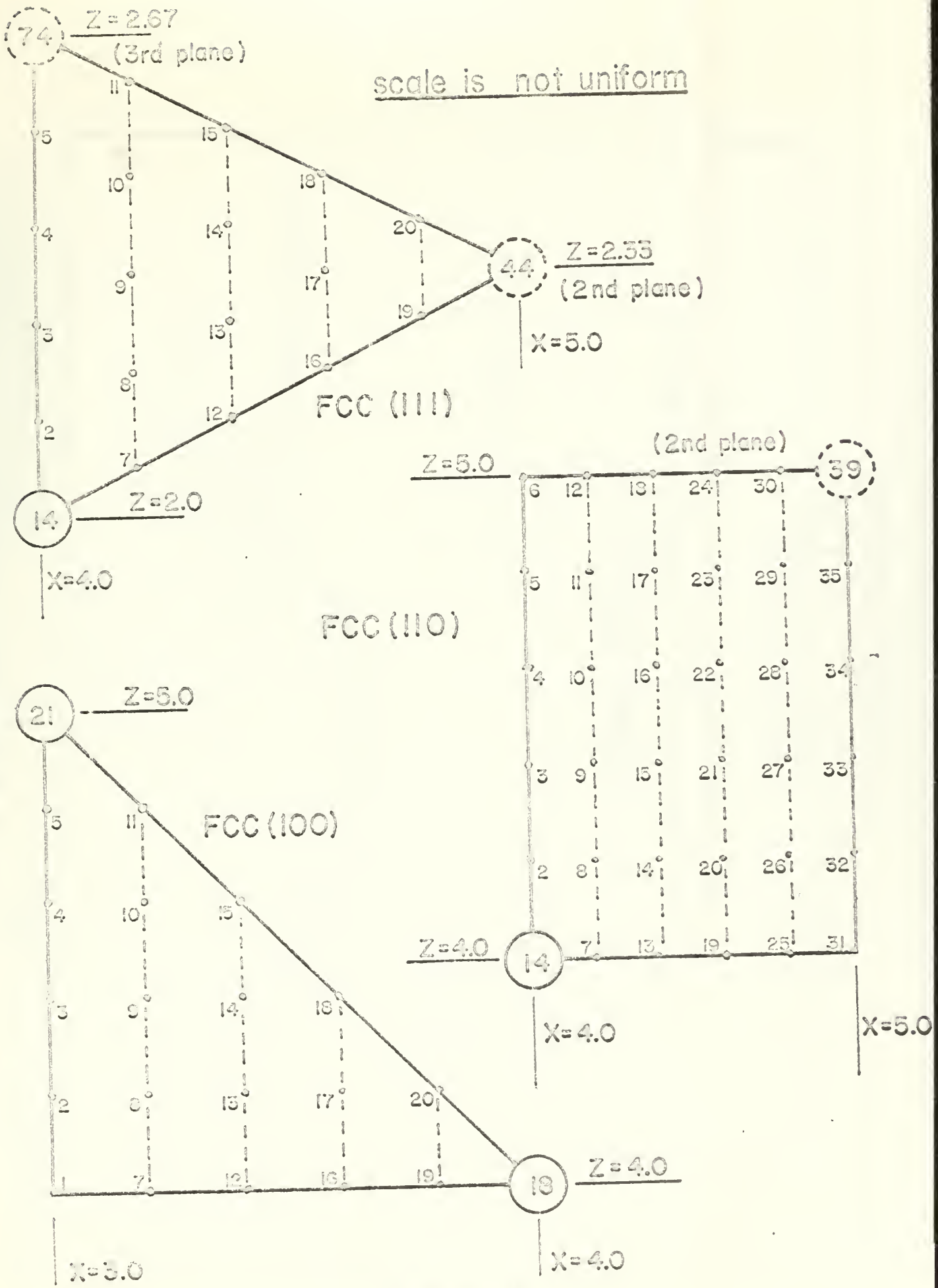

scale is not uniform
74
Z = 2.67
(3rd plane)
44
Z = 2.33
(2nd plane)
X = 5.0
14
Z = 2.0
X = 4.0
FCC (111)
(2nd plane)
Z = 5.0
39
Z = 4.0
14
X = 4.0
X = 5.0
FCC (110)
21
Z = 5.0
FCC (100)
18
Z = 4.0
X = 3.0
X = 4.0

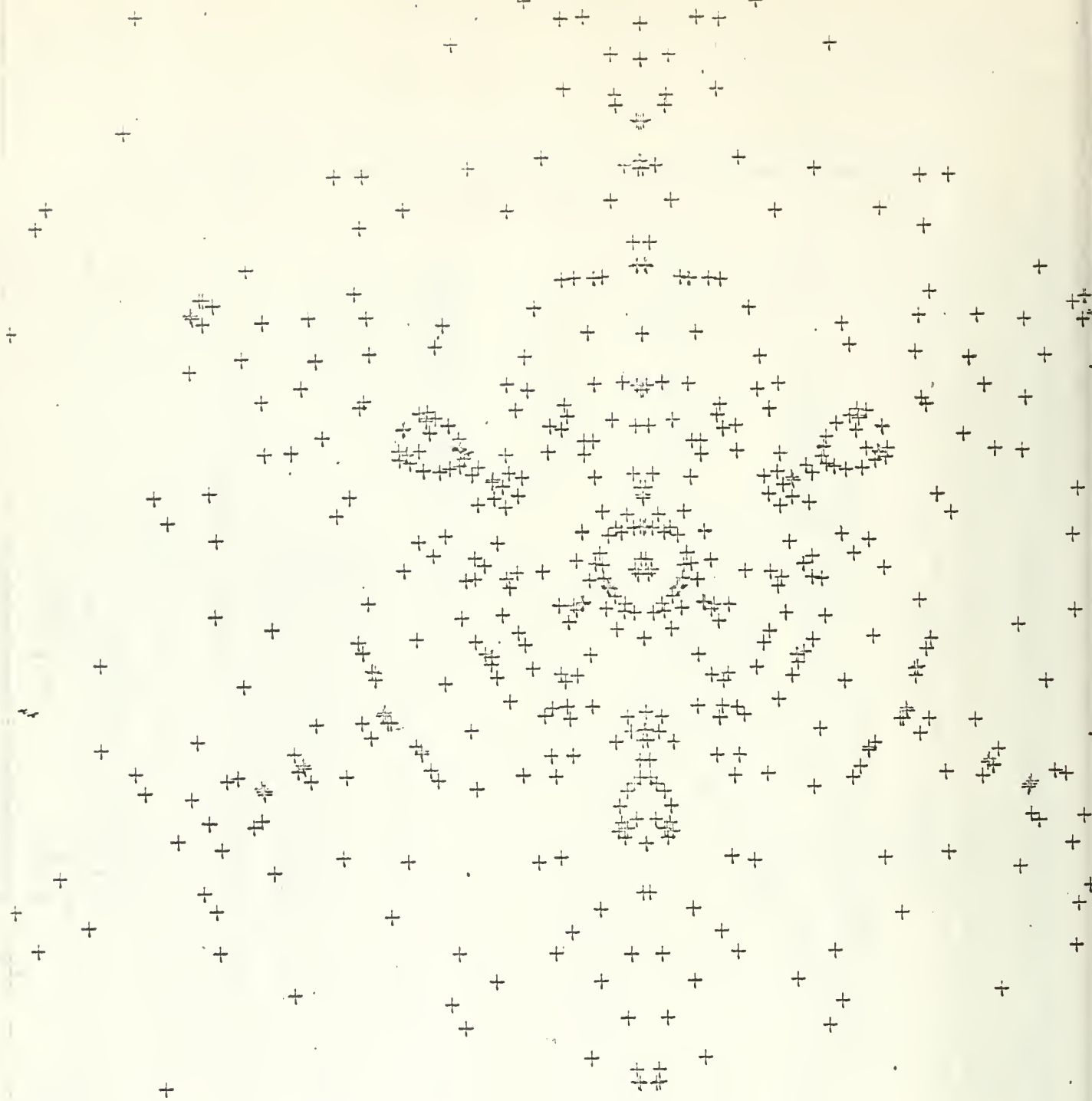
Figure 5

Argon-Copper
(111) orientation 10 KeV primary
Sputtering Ratio vs. "A" Potential Parameter
Regular Surface
"B" = -7.597
3 eV Binding Energy
4 eV
5 eV
10 eV
Sputtering Ratio (atoms/incident ion)
"A" Potential Parameter
1
2
3
11
12
13
14

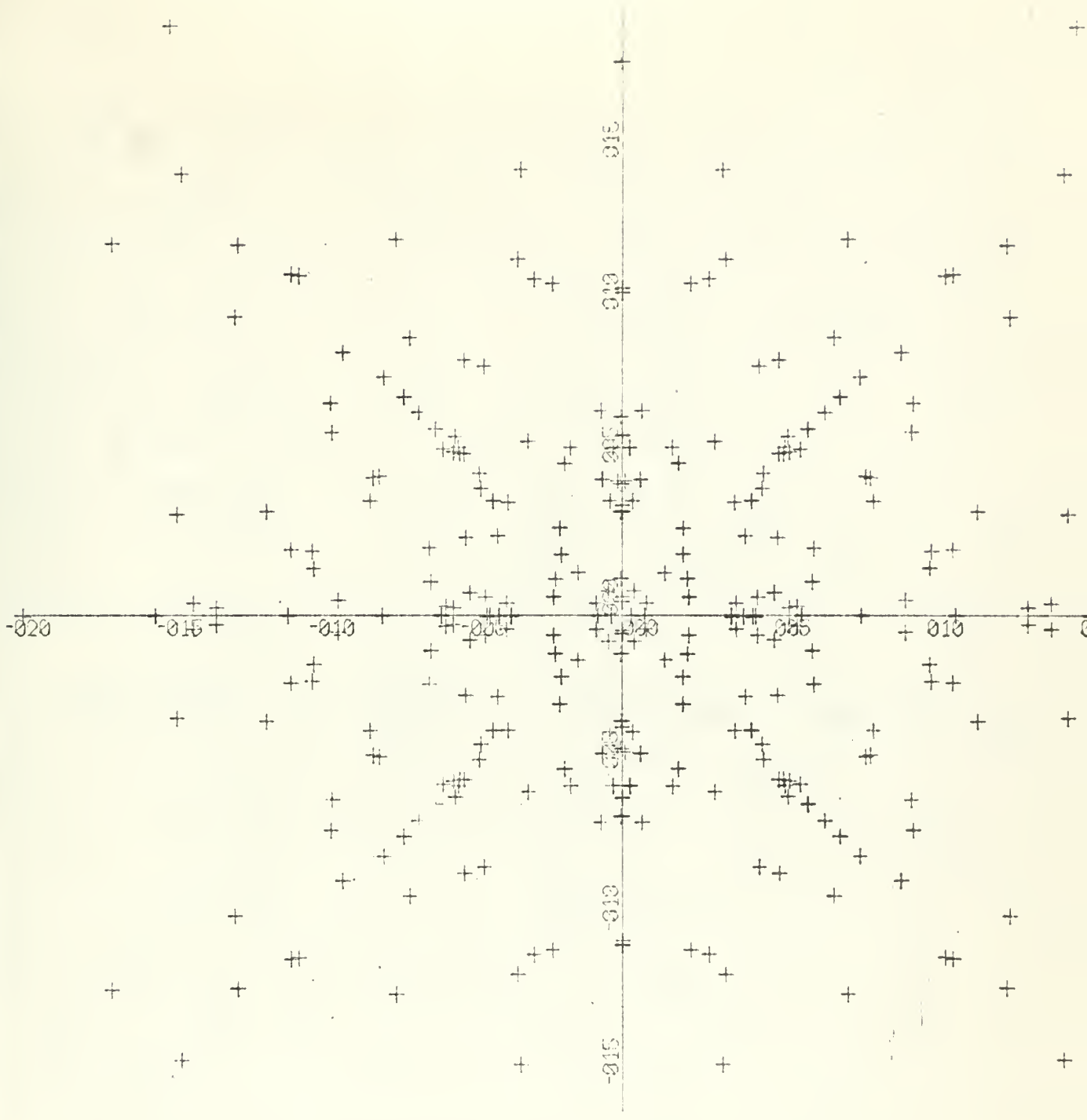
Figure 6

Argon-Copper
(111) orientation 10 KeV primary
Sputtering Ratio vs. "B" Potential Parameter
Regular Surface
"A" = 12.25
1 eV Binding Energy
3 eV
4 eV
10 eV
5
4
3
2
-7.7
-7.6
-7.5
"B" Potential Parameter
Sputtering Ratio (atoms/incident ion)

Figure 7



Argon-Copper Deposit Pattern
(111) orientation 7 KeV primary
Regular Surface
Scale=0.5 units/inch
Figure 8



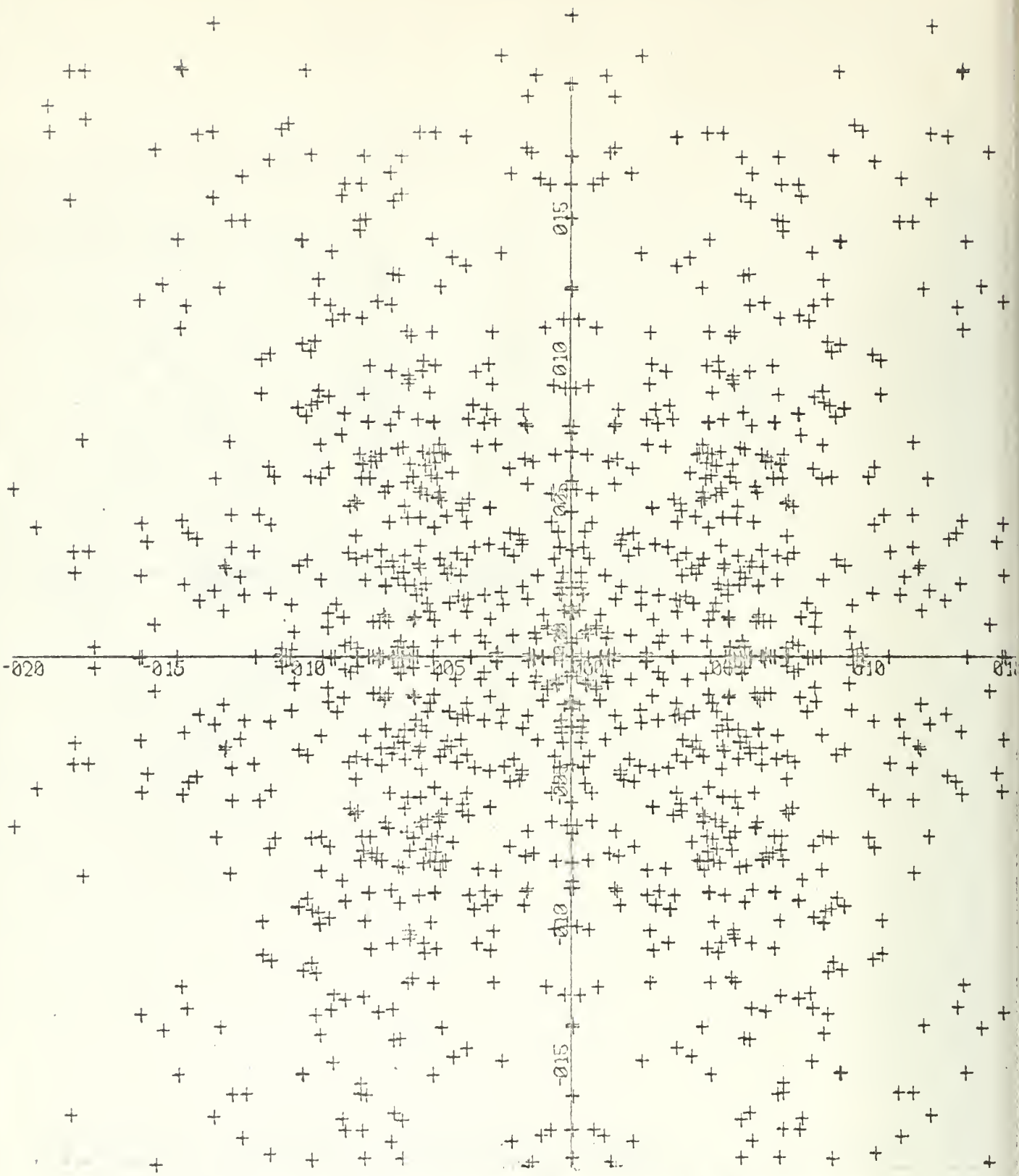
Argon-Copper Deposit Pattern

(100) orientation 10 KeV primary

Regular Surface

Scale = 0.5 units/inch

Figure 9



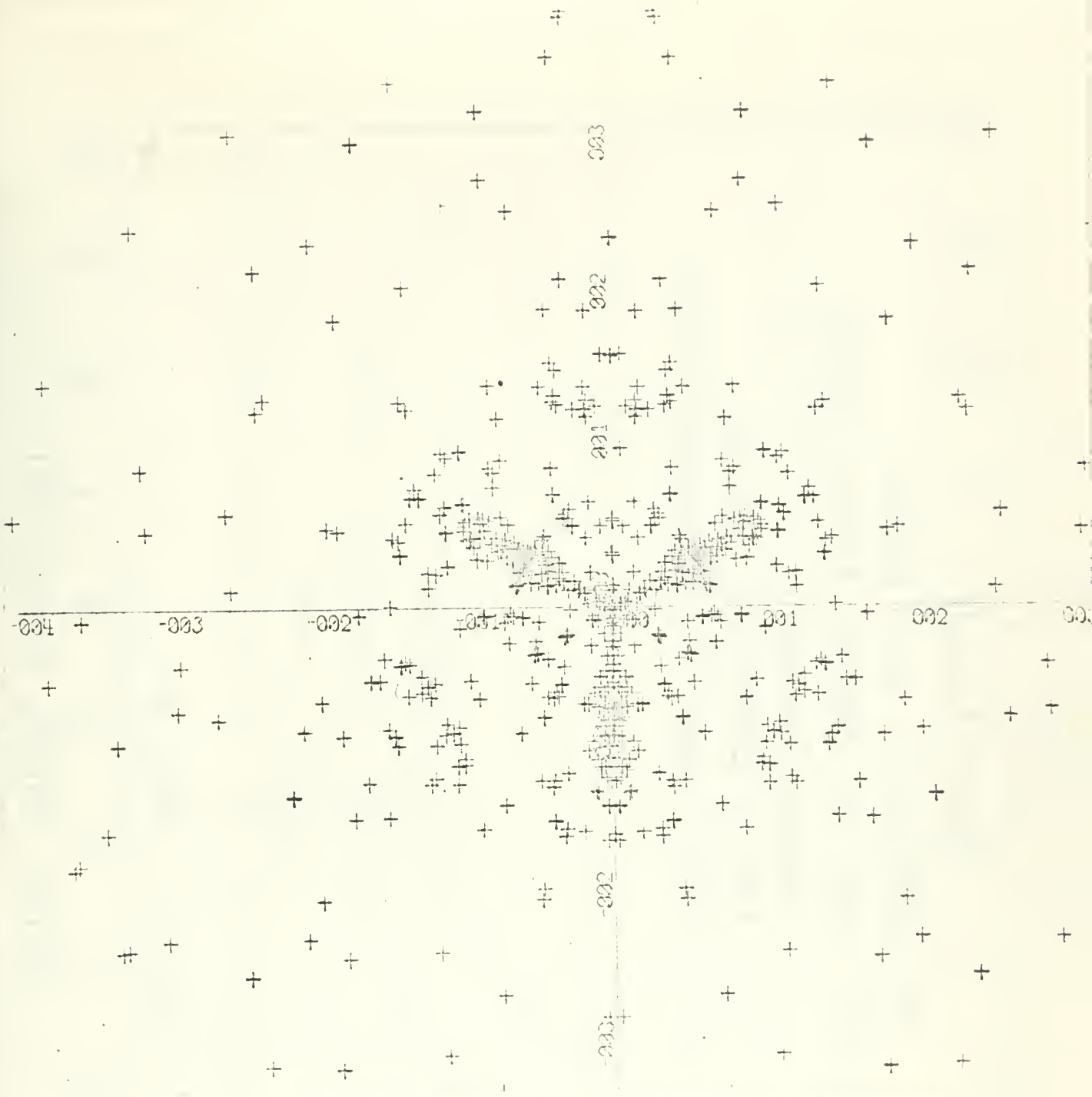
Argon-Copper Deposit Pattern

(110) orientation 3 KeV primary

Composite Surface

Scale = 0.5 units/inch

Figure 10



Argon-Copper Deposit Pattern

(III) orientation 3 KeV primary

One potential - Gibson 2

Regular Surface

Scale = 1.0 units/inch

Figure 11

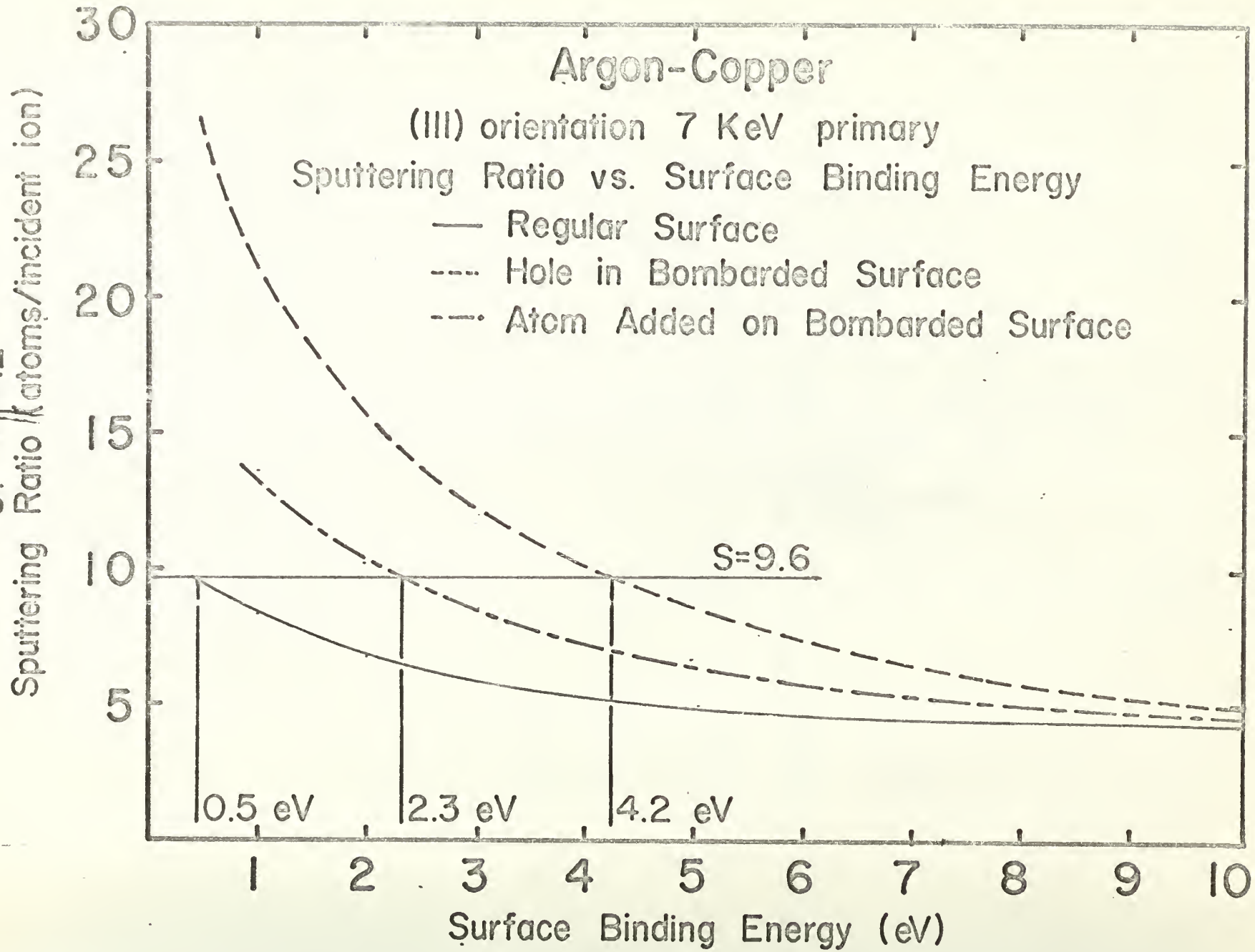

Argon-Copper
(III) orientation 7 KeV primary
Sputtering Ratio vs. Surface Binding Energy
Regular Surface
Hole in Bombarded Surface
Atom Added on Bombarded Surface
S=9.6
0.5 eV
2.3 eV
4.2 eV
Sputtering Ratio (atoms/incident ion)
Surface Binding Energy (eV)
30
25
20
15
10
5
1
2
3
4
5
6
7
8
9
10

Figure 12

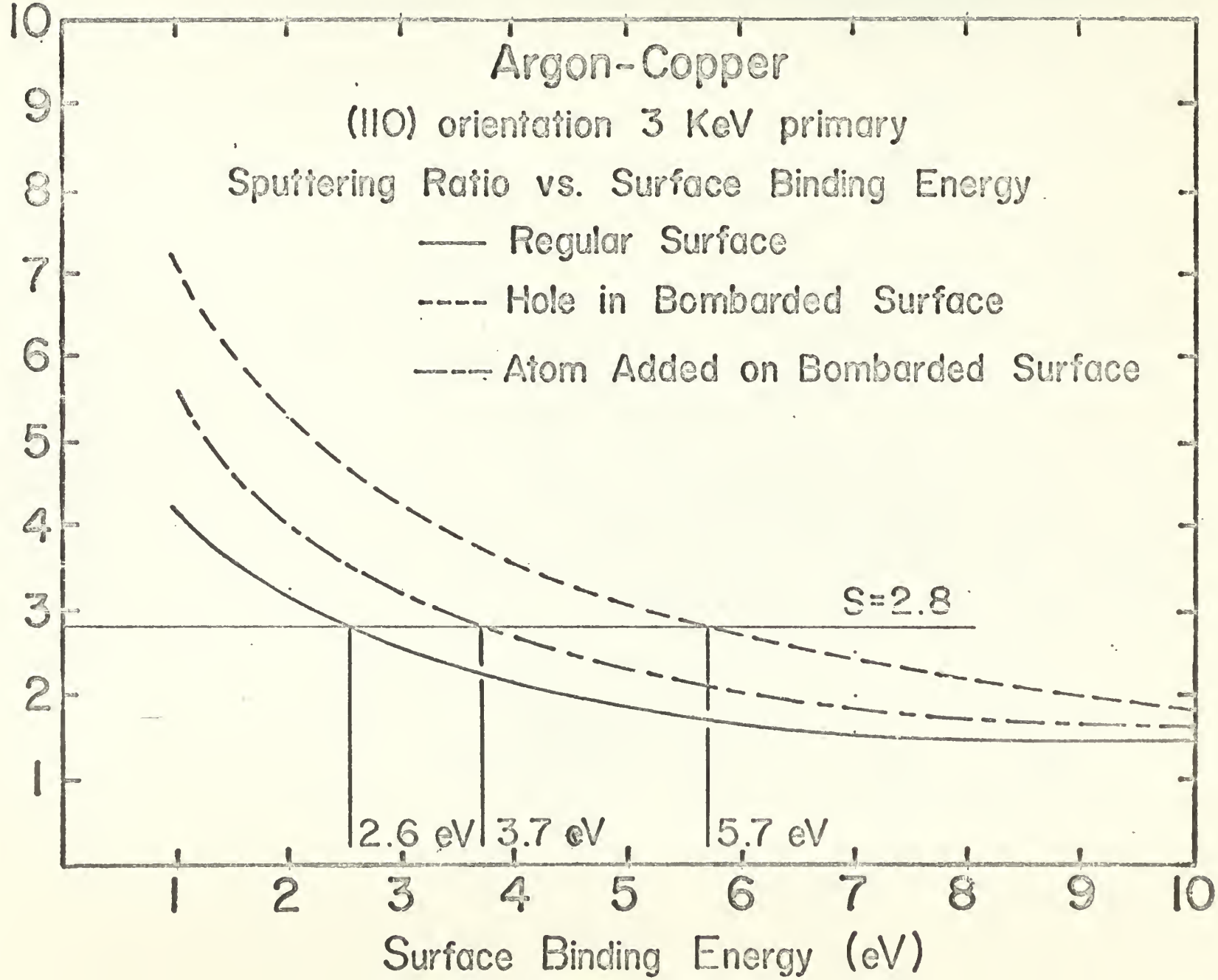
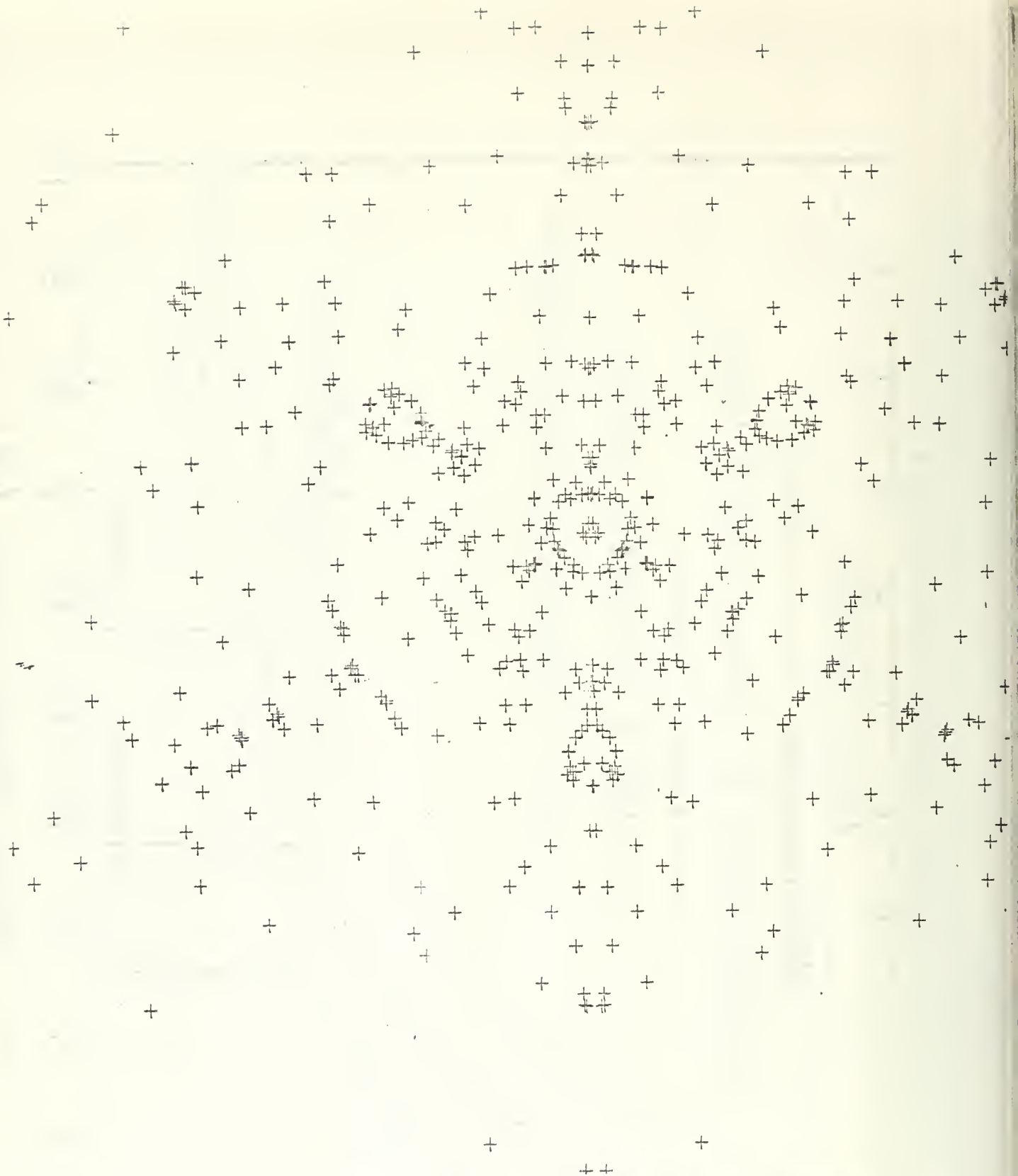
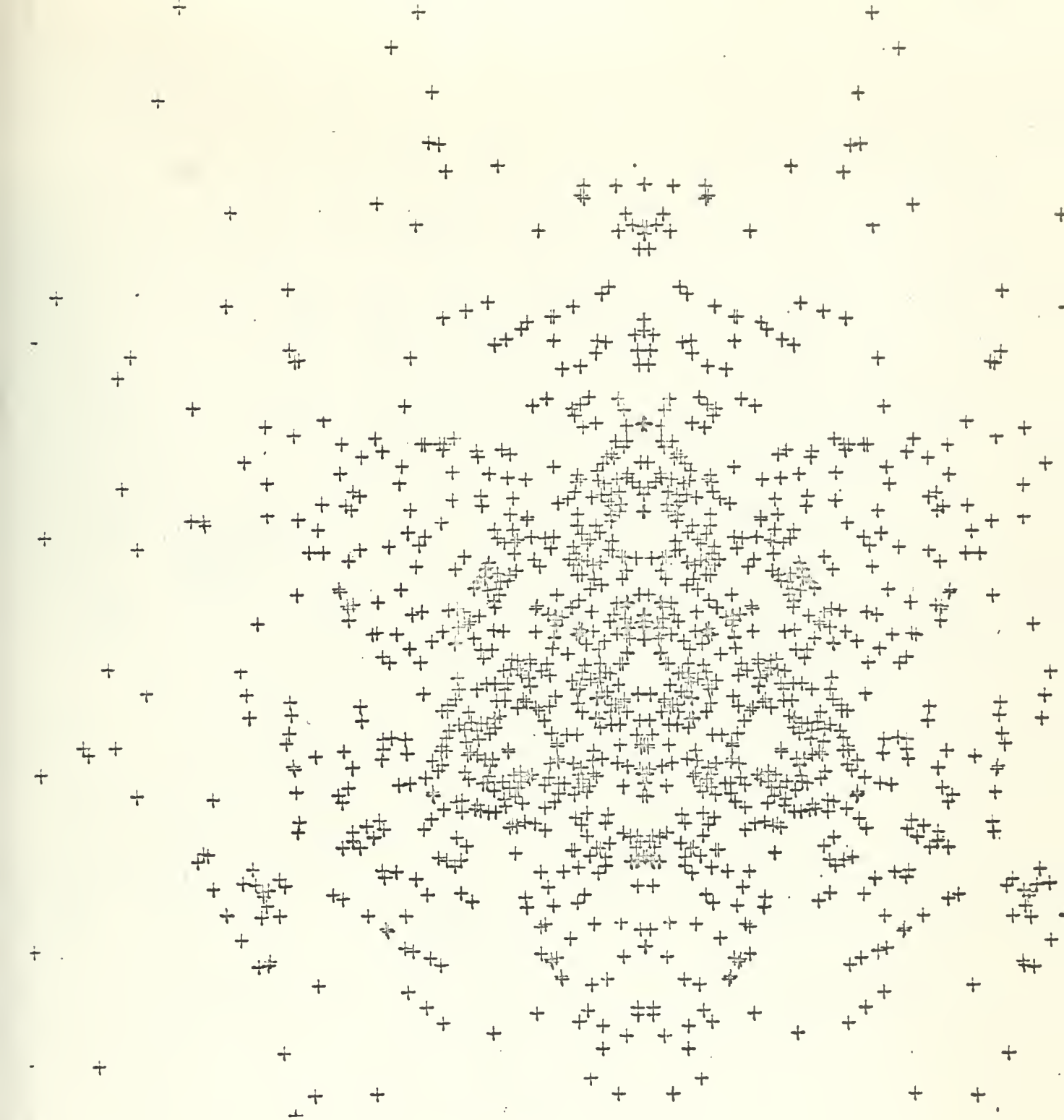

Argon-Copper
(110) orientation 3 KeV primary
Sputtering Ratio vs. Surface Binding Energy
—— Regular Surface
---- Hole in Bombarded Surface
—·— Atom Added on Bombarded Surface
S=2.8
2.6 eV
3.7 eV
5.7 eV
Sputtering Ratio (atoms/incident ion)
Surface Binding Energy (eV)
1
2
3
4
5
6
7
8
9
10

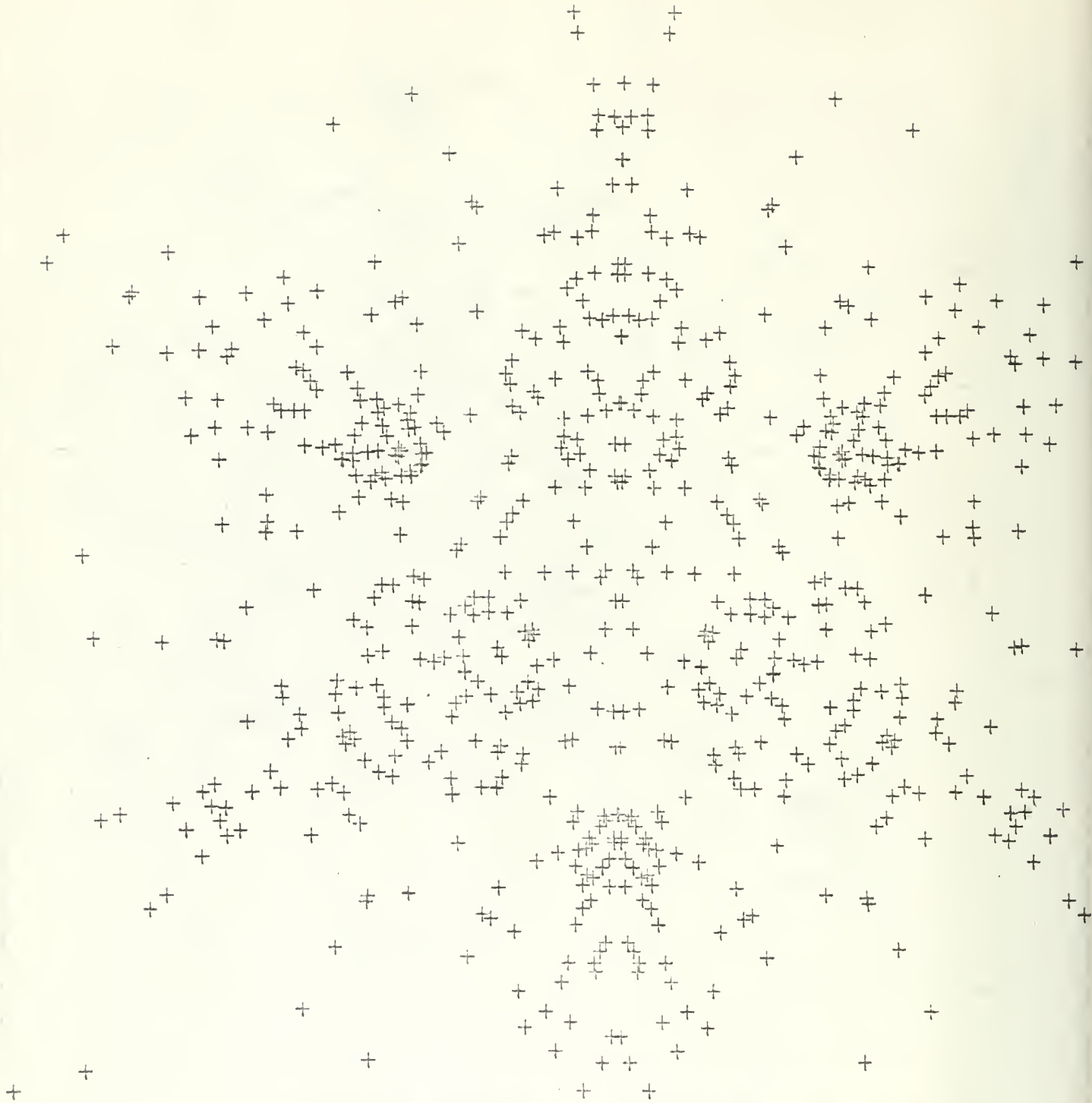
Figure 13



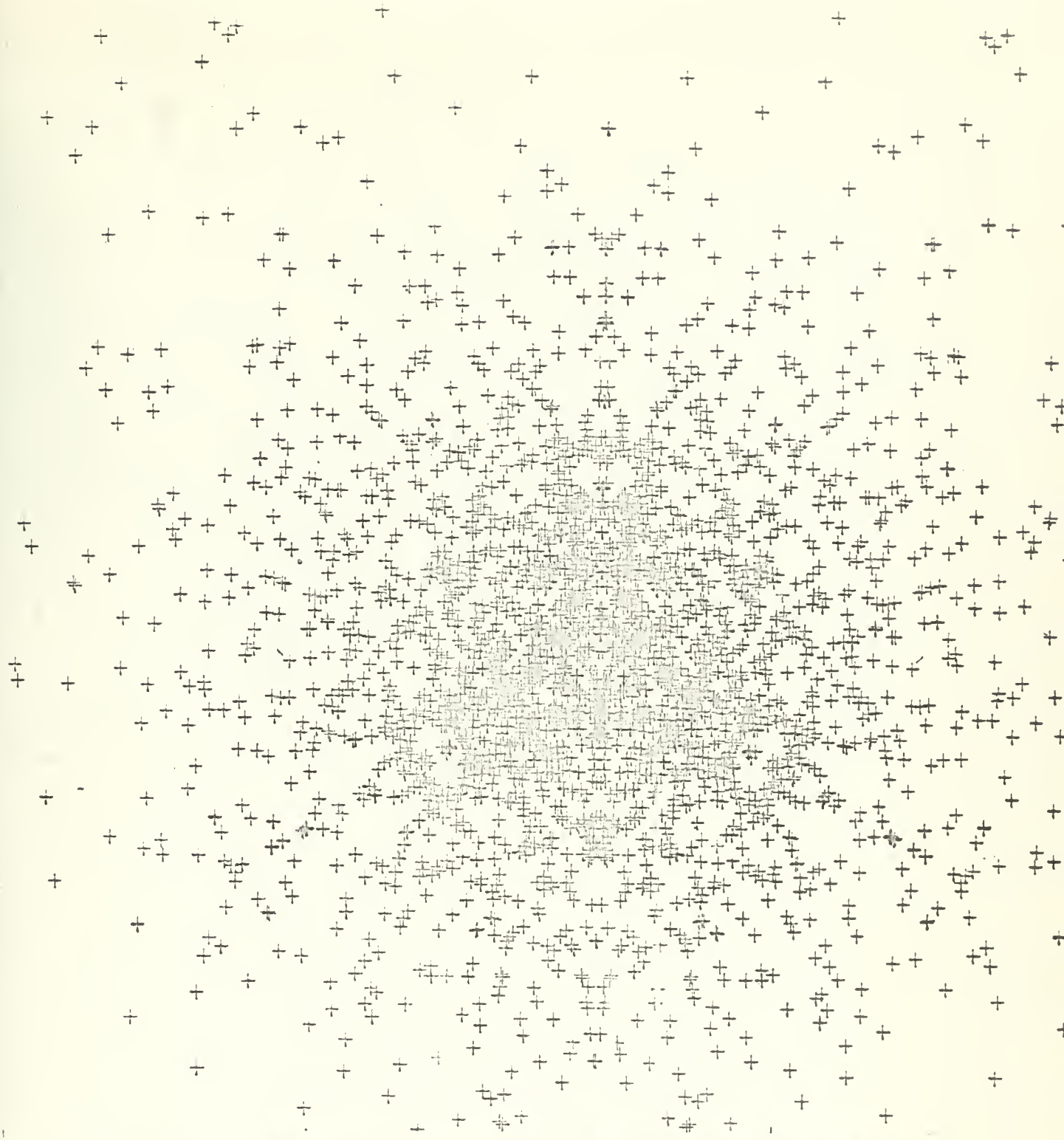
Argon-Copper Deposit Pattern
(111) orientation 7 KeV primary
Regular Surface
Scale = 0.5 units/inch
Figure 14



Argon-Copper Deposit Pattern
(111) orientation 7 KeV primary
Hole in Bombarded Surface
Scale=0.5 units/inch
Figure 15



Argon-Copper Deposit Pattern
(III) orientation 7 KeV primary
Atom Added on Bombarded Surface
Scale=0.5 units/inch
Figure 16



Argon-Copper Deposit Pattern

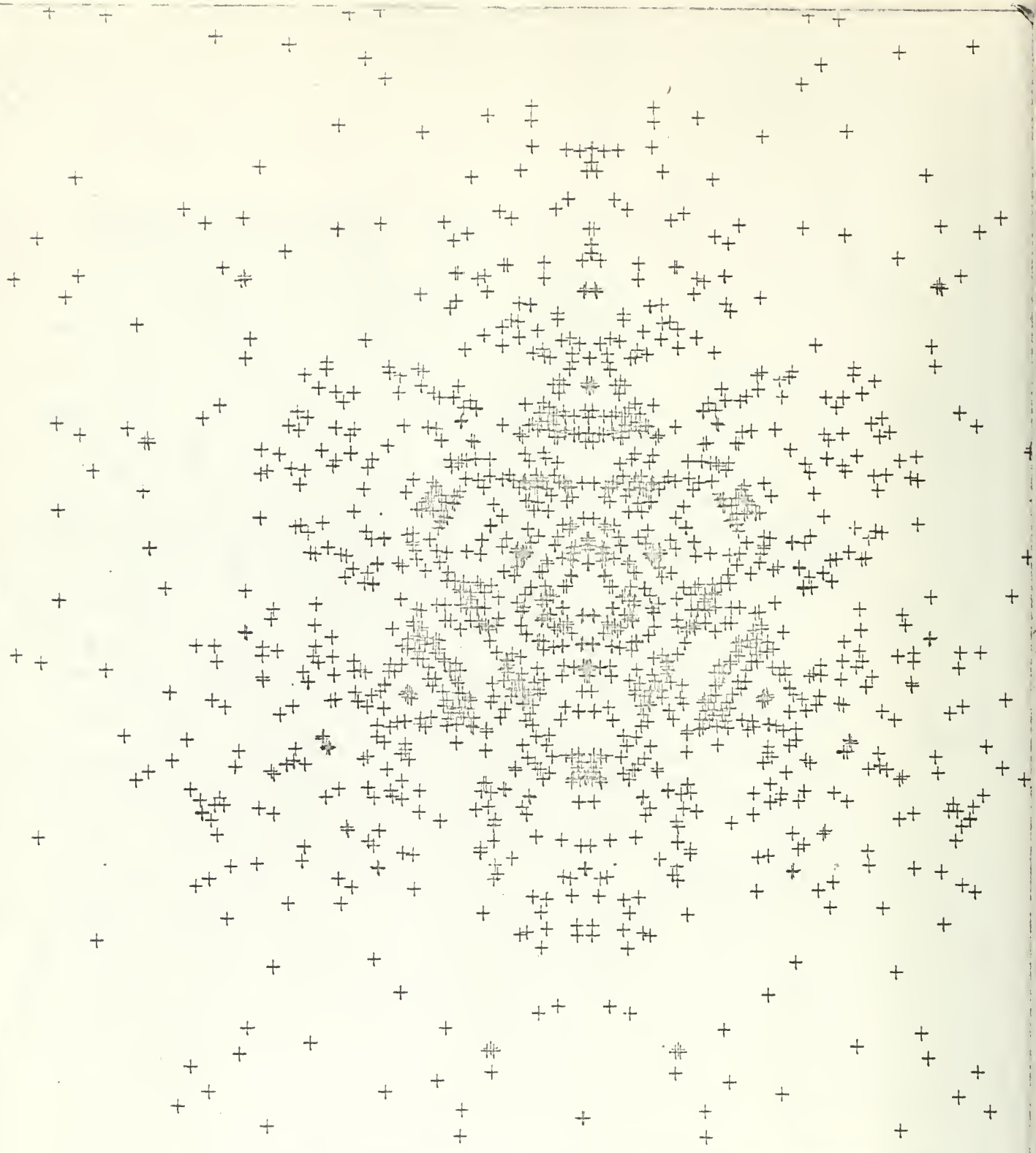
(111) orientation 7 KeV primary

Hole in Bombarded Surface

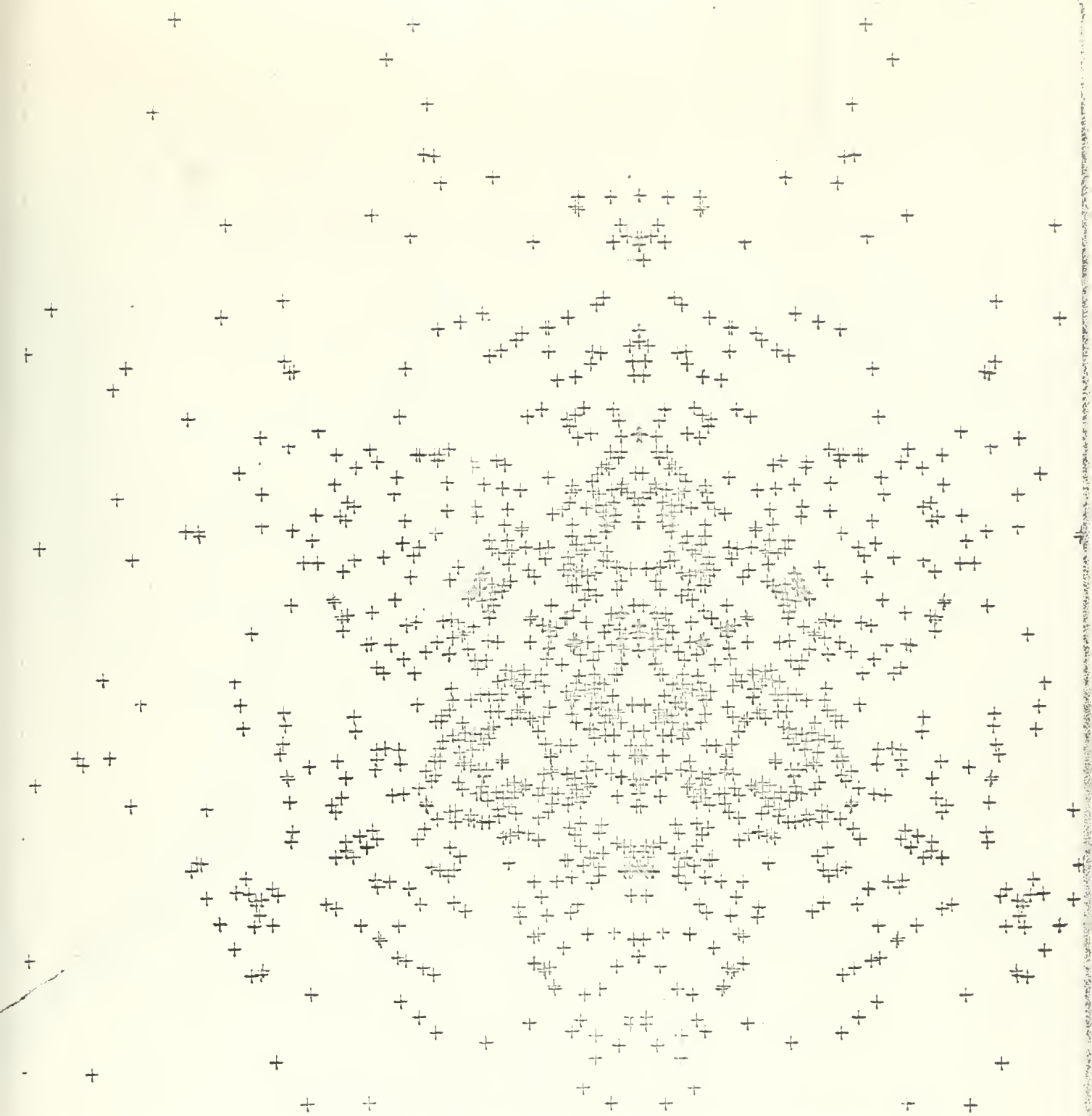
Surface Binding Energy = 0.5 eV

Scale = 0.5 units/inch

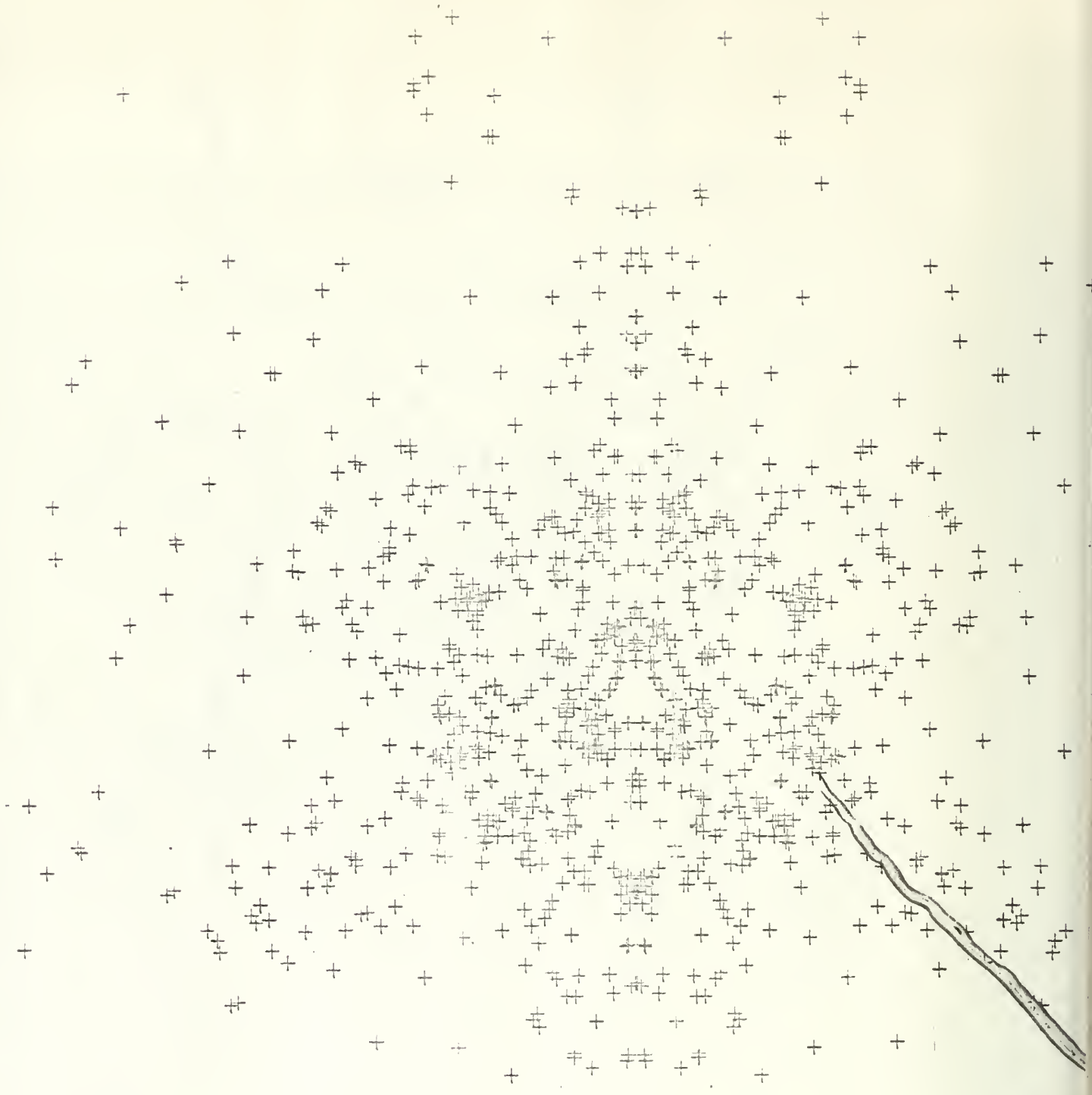
Figure 17



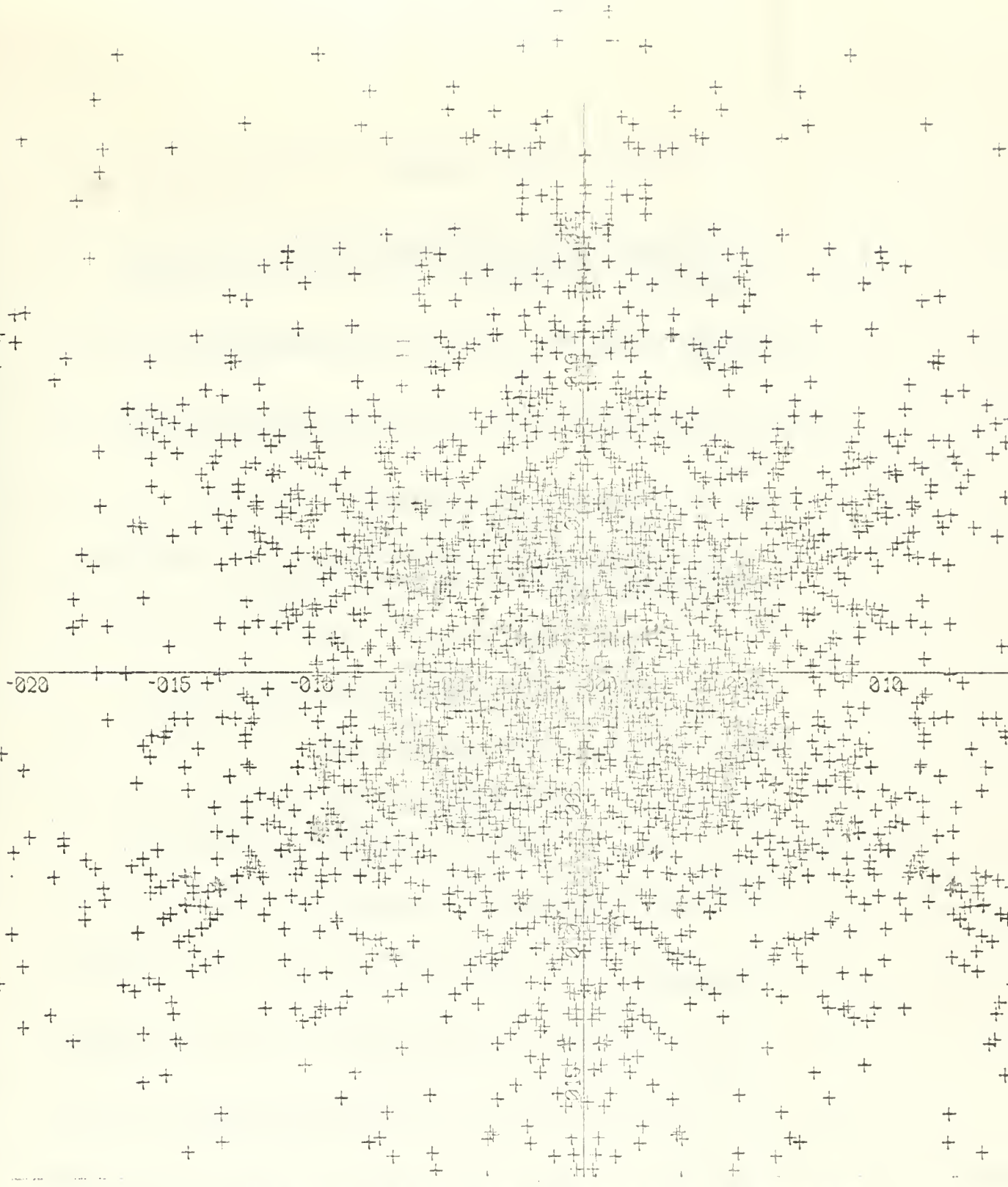
Argon--Copper Deposit Pattern
(111) orientation 7 KeV primary
Hole in Bombarded Surface
Surface Binding Energy = 2.0 eV
Scale = 0.5 units/inch
Figure 18



Argon-Copper Deposit Pattern
(111) orientation 7 KeV primary
Hole in Bombarded Surface
Surface Binding Energy = 2.5 eV
Scale = 0.5 units/inch
Figure 19



Argon-Copper Deposit Pattern
(111) orientation 7 KeV primary
Hole in Bombarded Surface
Surface Binding Energy = 4.0 eV
Scale = 0.5 units/inch
Figure 20



Argon-Copper Deposit Pattern

(111) orientation 7 KeV primary

Composite Surface

Surface Binding Energy = 2.25 eV

Scale = 0.5 units/inch

Figure 21

BIBLIOGRAPHY

1. W. R. Grove, Philosophical Transactions of the Royal Society 142, 87 (1852).

2. K. H. Kingdon and J. Langmuir, Physical Review 22, 148 (1923).

3. E. Blechschmidt and A. von Hippel, Annalen der Physik 86, 1006 (1928).

4. C. H. Townes, Physical Review 65, 319 (1944)

5. N. Bohr, Kgl. Dnaske Videnskabernes Selskab, Mathematisk-fysike Meddelelser 18, No. 8, (1948).

6. F. Keywell, Physical Review 97, 1611 (1955).

7. D. E. Harrison, Physical Review 102, 1473 (1956).

8. D. E. Harrison, Physical Review 105, 1212 (1957).

9. G. K. Wehner, Physical Review 102, 690 (1956).

10. E. B. Henschke, Physical Review 106, 737 (1957).

11. E. Lanberg, Physical Review 111, 91 (1958).

12. J. B. Gibson, A. N. Goland, M. Milgram, and G. Vineyard, Physical Review 120, 1229 (1961).

13. O. S. Oen and D. K. Holmes, and M. T. Robinson, Journal of Applied Physics 34, 302 (1963).

14. M. T. Robinson and O. S. Oen, Physical Review 132, 2385 (1963).

15. O. S. Oen and M. T. Robinson, Journal of Applied Physics 35, 2515 (1964).

16. C. Erginsoy, G. H. Vineyard, and A. Englert, Physical Review 133, A595 (1964).

17. W. L. Gay and D. E. Harrison, Physical Review 135, A1780 (1964).

18. N. S. Levy, Computer Simulation of the Sputtering Process. Thesis, U. S. Naval Postgraduate School (unpublished).

19. G. D. Magnuson and C. E. Carlston, Physical Review 129, 2409 (1963).

20. D. E. Harrison Jr., and C. E. Carlston and G. D. Magnuson, Physical Review 139, A737 (1965).

21. C. E. Carlston, G. D. Magnuson, P. Mahadevan, and D. E. Harrison, Jr., Physical Review 139, A729 (1965).

22. G. S. Anderson and G. K. Wehner, Journal of Applied Physics 31, 2305 (1960).

23. A. L. Southern, W. R. Willis, and M. T. Robinson, Journal of Applied Physics 34, 153 (1963).

24. R. H. Silsbee, Journal of Applied Physics 28, 1246 (1957).

25. D. E. Harrison, Jr., J. P. Johnson III, and N. S. Levy, Applied Physics Letters 8, 33 (1966).

26. G. D. Magnuson and C. E. Carlston, Journal of Applied Physics 34, 3267 (1963).

APPENDIX I

PROGRAM LISTING

A. TWOPOT LISTING

SECTION 1

```
      PROGRAM TWOPOT
C
C THIS DECK INVESTIGATES THE SPUTTERING PROCESS WHEN THE TARGET ATOM,
C NUMBER 93, HAS BEEN REMOVED.
C THIS PROGRAM CONSTRUCTS THE MICROCRYSTALLITE AND INTEGRATES THE
C FORCE LAWS FOR THE (111) ORIENTATION
C THIS DECK PRODUCES THE LEFT HAND PORTION OF THE CRYSTAL. ATOMS
C NUMBERED 2 THROUGH 151.
C
      POTF(X)=EXPF(EXA+EXB*X)
      FORC(X)=EXPF(FXA+EXB*X)
      PPOTF(X)=EXPF(PEXA+PEXB*X)
      PFORCF(X)=EXPF(PFXA+PEXB*X)
      DIMENSION RX(500),RY(500),RZ(500),FX(1000),FY(1000),FZ(1000)
      DIMENSION KCUT(500)
      DIMENSION LCUT(500)
      DIMENSION VX(1000),VY(1000),VZ(500)
      DIMENSION PKEY(500)
      DIMENSION PPE(1000),PKE(1000),PTE(1000)
      DIMENSION RXK(1000),RYK(1000),RZK(1000)
      DIMENSION RXI(1000),RYI(1000),RZI(1000)
      DIMENSION DX(1000),DY(1000),DZ(1000)
      DIMENSION IH(5)
      COMMON RXK,RYK,RZK,RXI,RYI,RZI
      EQUIVALENCE (DX,RXK),(DY,RYK),(DZ,RZK)
      LOC(ILIM=57B,INOW=50B)
 9000 FORMAT(1H )
 9001 FORMAT(1H1)
 9010 FORMAT(80H
     1                              /)
 9011 FORMAT(4F10.5,5A8)
```

```
9012 FORMAT(/,29H BULLET INCOMING LOCATION  X= F6.3, 5H   Z= F6.3,
    110H   ENERGY= F10.1,24H   TIME STEP MULTIPLIER=  F5.3, /  )
9014 FORMAT(5H EXA=,F9.5,6H  EXB=,F9.5,6H  FXA=,F9.5,16H  LATTICE UNIT
    1=,F5.3,15H ANGSTROM UNITS,5X,17H BINDING ENERGY =,F5.1,3H EV,/)
9015 FORMAT(36X,6H PEXA=,F9.5,6H PEXB=,F9.5,6H PFXA=,F9.5,/)
9016 FORMAT(40X,5A8,/)
9017 FORMAT(2F10.5)
9020 FORMAT(1I8,3F10.5,3E10.2,4F10.4 )
9030 FORMAT(107H     ATOM    DX         DY         DZ         VX         VY
    1         VZ         KE         PE         TE       KE(Y)      /)
9040 FORMAT(2F8.3,3F5.2,E8.2,3F8.5,I5,2I3,I2,A4)
9050 FORMAT(36X,14H BULLET MASS= ,F7.3,15H TARGET MASS=  ,F7.3,10X,16HP
    1OSITION NUMBER ,A4,/)
9060 FORMAT(22H ELAPSED TIME (SEC) = ,E10.4,19H   THERMAL CUTOFF =,F5.3
    1,3H EV,22H ENERGY LOSS CONSTANT=,1PE10.3,0P,11H TIMESTEP =,I6,//)
9070 FORMAT(1X,F10.3,24H EV,TOTAL KINETIC ENERGY,,F10.3,27H EV,TOTAL PO
    1TENTIAL ENERGY,F10.3,17H EV,TOTAL ENERGY   )
9080 FORMAT(36X,14H COSINE TO X =,F7.5,16H,  COSINE TO Y =,F7.5,/)
9090 FORMAT(29H TARGET POINT ON CRYSTAL   X=,F6.3, 5H   Z= F6.3,28H   C
    1UTOFF ENERGY THRESHOLD =,F6.1,15H  SAMPLE SIZE (,I3,2H X,I3,2H X,
    2I3,2H ),/)
9091 FORMAT(3I5,2E20.11,3F8.2,/)
9092 FORMAT(I4,3F12.8,3E16.9,2F10.4,I2)
9093 FORMAT(105X,4HPAGE,I3,/,1H1)
9094 FORMAT(I4,3F7.2,3F7.2,3E9.2,3F5.2,1F8.2,2I4)
9095 FORMAT(121H ATOM  RX     RY     RZ     DX     DY     DZ     VX
    1   VY       VZ    DCOSXDCOSYDCOSZ  PKEY LCUT  KCUT
    1/)
9096 FORMAT(118H ATOM     RX          RY          RZ          VX
    1          VY               VZ          PKE         PPE LCUT      /)
```

```
      MASK=77777777777777778
      THERM=0.25
      FM=1.0E-10
      QUIT=0.5
      SLOW=0.5E-12
      ZE=0.0
      EI=25.0
      CVE=1.60E-19
      CVM=1.672E-27
      READ INPUT TAPE 2,9010
      READ INPUT TAPE 2,9011,EXA,EXB,CVR,CVS,IH
      READ INPUT TAPE 2,9017,PEXA,PEXB
      CELS=-CVS*1.0E-13
      CVD=CVR*1.0E-10
      FXA=LOGF(-EXB*CVE/CVD)+EXA
      ROE2=2.0
      ROE=SQRTF(ROE2)
      FRC=FORC(ROE)
      PTC=POTF(ROE)
      PFXA=LOGF(-PEXB*CVE/CVD)+PEXA
      PFRC=PFORCF(ROE)
      PPTC=PPOTF(ROE)
      CVB=0.774E-9
      BENERGY=2.0
      WRITE OUTPUT TAPE 3,9001
    4 READ INPUT TAPE 2,9040,GMAS,TMAS,BX,BY,BZ,EV,DTI,COX,COY,NTT,NS,ND
     1,NRS,PNUM
      LDA(GMAS),AJP3(9999).
      INDEX = 0
      ROEM=ROE-DTI
      FRC=PTC/DTI
      PFRC=PPTC/DTI
      PGMAS=GMAS*CVM
      PTMAS=TMAS*CVM
      HGMAS=0.5*PGMAS/CVE
      HTMAS=0.5*PTMAS/CVE
      RXBOUND=6.36396103
      RZBOUND=6.94022094
      RYBOUND=4.61880215
```

```
      IX=10
      IY=5
      IZ=6
      IXP=(IX+1)/2
      IYP=(IY+1)/2
      IZP=(IZ+1)/2
      M=2
      SCX=1.0/ROE
      SCY=ROE2/SQRTF(3.0)
      SCZ=SQRTF(1.5)
      SSCZ=SCZ/3.0
C
C THIS PACKAGE CONSTRUCTS THE CRYSTAL FIRST IN THE Z-DIRECTION, THEN
C THE Y-DIRECTION AND THEN IN THE X-DIRECTION
C
      IT=
      X=-SCX
      DO 60 I=1,IX
      X=X+SCX
      JT=
      Y=-SCY
      DO 59 J=1,IY
      Y=Y+SCY
      Z=-SCZ
      KT=
      JTS=JT+JT/3
      DO 58 K=1,IZ
      Z=Z+SCZ
      LDA(IT)ADD(JTS)ADD(KT)ENQ(0)LRS(1)QJP3(57)
      X=IT
      RX(M)=X*SCX
      RY(M)=Y
      IF(JT-3*(JT/3)) 41,42,41
```

```
41 LDA(JT)+INA(-3)+AJP2(L-1)INA(3)STA(JTT)
   X=JTT
    RZ(M)=X*SSCZ
   X=KT
    RZ(M)=RZ(M)+X*SCZ
   GO TO 49
42 X=KT
    RZ(M)=X*SCZ
49 M=M+1
57 KT=KT+1
58 CONTINUE
   JT=JT+1
59 CONTINUE
   IT=IT+1
60 CONTINUE
   LL=M-1
   DO 63 I=2,LL
   VX(I) = 0.0
   VY(I) = 0.0
   VZ(I) = 0.0
63 CONTINUE
```

```
      VOL=SQRTF(EV/HGMAS)
      VX(1)=VOL*COX
      VY(1)=VOL*COY
      TIME=BY/VY(1)
      COZ=1.0-COX*COX-COY*COY
      COZ=ABSF(COZ)
      COZ=SQRTF(COZ)
      VZ(1)=VOL*COZ
      RX(1)=SCX*BX+TIME*VX(1)
      RY(1)=BY
      RZ(1)=SCZ*BZ+TIME*VZ(1)
      DO 66 I=1,LL
      KCUT(I)=0
      LCUT(I)=0
      RXI(I)=RX(I)
      RYI(I)=RY(I)
   66 RZI(I)=RZ(I)
   69 DT=DTI*CVD/VOL
      DXS=0.0
      DYS=0.0
      DZS=0.0
      TIME=0.0
      NT=
      NL=
      NSHUT=0
      NLDTI=1.0/DTI
      ENI5(0)ENI6(0)
      NPAGE=1
   68 DTOD=DT/CVD
      HDTOM=0.5*DT/PTMAS
      QDTOM=0.5*HDTOM
      HDTOMB=0.5*DT/PGMAS
      QDTOMB=0.5*HDTOMB
```

```
 70 DO 75 I=1,LL
 75 LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
    LDA(ZE)STA(TPOT)STA(TPKE)STA(SPE)
105 LDA(LL)SAU(L+2)ENI1(0)ENI(0)
110 ISK1(*)SLJ(L+2)SLJ(200)ENI(0)
    LDA1(LCUT)AJP1(110)
    LDA(LL)SAU(L+3)
    ENA1(0)SAL(IP1)LIL2(IP1)ENI(0)
120 ISK2(*)SLJ(L+2)SLJ(110)ENI(0)
    LDA2(LCUT)AJP1(120)
    DRX = RX(J) - RX(I)
    +SSK(DRX),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
    DRY=RY(J)-RY(I)
    +SSK(DRY),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
    DRZ=RZ(J)-RZ(I)
    +SSK(DRZ),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
150 LDA(DRX)FMU(DRX)STA(DIST)LDA(DRY)FMU(DRY)FAD(DIST)STA(DIST)LDA(DRZ
   1)FMU(DRZ)FAD(DIST)STA(DIST)FSB(ROE2)AJP2(120)
155 DIST = SQRTF( DIST)
    ENA1(0)INA(-1)AJP1(170)ENI(0)
    LDA(ROEM)FSB(DIST)AJP3(166)ENI(0)
    FORCE=PFORCF(DIST)
    GO TO 180
166 FORCE=PFORCF(DIST)-PFRC
    GO TO 180
170 LDA(ROEM)FSB(DIST)AJP3(175)ENI(0)
    FORCE=FORC(DIST)
    GO TO 180
175 FORCE=FORC(DIST)-FRC
180 LDA(FORCE)FSB(FM)AJP3(120)
    FOD = FORCE / DIST
    FA = DRX * FOD
    FB = DRY * FOD
    FC = DRZ * FOD
```

```
160 FX(J) = FX(J) + FA
    FY(J) = FY(J) + FB
    FZ(J) = FZ(J) + FC
165 FX(I) = FX(I) - FA
    FY(I) = FY(I) - FB
    FZ(I) = FZ(I) - FC
    SLJ(120)
200 CONTINUE
    LDA(LL)SAU(L+2)ENI1(1)ENI(0)
211 ISK1(*)SLJ(L+2)SLJ(220)ENI(0)
    LDA1(RY)AJP3(214)
    SLJ(211)
214 FAD(SCY)AJP3(211)AJP(211)
    LDA1(FY)FAD(BIND)STA1(FY)
    SLJ(211)
220 LDA(INDEX)AJP1(260)
    INDEX=1
    I=1
    RXK(I)=RX(I)
    RYK(I)=RY(I)
    RZK(I)=RZ(I)
    RX(I)=(VX(I)+FX(I)*HDTOMB)*DTOD+RX(I)
    RY(I)=(VY(I)+FY(I)*HDTOMB)*DTOD+RY(I)
    RZ(I)=(VZ(I)+FZ(I)*HDTOMB)*DTOD+RZ(I)
    DO 250 I=2,LL
    RXK(I)=RX(I)
    RYK(I)=RY(I)
    RZK(I)=RZ(I)
    RX(I)=(VX(I)+FX(I)*HDTOM)*DTOD+RX(I)
    RY(I)=(VY(I)+FY(I)*HDTOM)*DTOD+RY(I)
    RZ(I)=(VZ(I)+FZ(I)*HDTOM)*DTOD+RZ(I)
250 CONTINUE
    GO TO 105
260 INDEX=0
    TIME=TIME+DT
    NT=NT+1
    NL=NL+1
```

```
      I=1
      RX(I)=RXK(I)+(VX(I)+FX(I)*QDTOMB)*DTOD
      RY(I)=RYK(I)+(VY(I)+FY(I)*QDTOMB)*DTOD
      RZ(I)=RZK(I)+(VZ(I)+FZ(I)*QDTOMB)*DTOD
      VX(I)=VX(I)+FX(I)*HDTOMB
      VY(I)=VY(I)+FY(I)*HDTOMB
      VZ(I)=VZ(I)+FZ(I)*HDTOMB
      LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
      DO 300 I=2,LL
      RX(I)=RXK(I)+(VX(I)+FX(I)*QDTOM)*DTOD
      RY(I)=RYK(I)+(VY(I)+FY(I)*QDTOM)*DTOD
      RZ(I)=RZK(I)+(VZ(I)+FZ(I)*QDTOM)*DTOD
      VX(I)=VX(I)+FX(I)*HDTOM
      VY(I)=VY(I)+FY(I)*HDTOM
      VZ(I)=VZ(I)+FZ(I)*HDTOM
      LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
  300 CONTINUE
```

SECTION 6

```
    LDA(LL)SAU(309)ENI1(1)ENI(0)
301 LDA1(KCUT)AJP(302)SLJ(309)ENI(0)
302 LDA1(RY)AJP3(308)FSB(RYBOUND)AJP3(L+3)
    AJP(L+2)LDA1(KCUT)INA(2)STA1(KCUT)
    LDA1(RX)AJP3(307)FSB(RXBOUND)AJP3(L+3)
    AJP(L+2)LDA1(KCUT)INA(4)STA1(KCUT)
    LDA1(RZ)AJP3(306)FSB(RZBOUND)AJP3(309)
    AJP(309)LDA1(KCUT)INA(6)STA1(KCUT)
    SLJ(309)ENI(0)
306 LDA1(KCUT)INA(5)STA1(KCUT)SLJ(309)
307 LDA1(KCUT)INA(3)STA1(KCUT)SLJ(309)
308 LDA1(KCUT)INA(1)STA1(KCUT)ENI(0)
309 ISK1(*)SLJ(301)
```

SECTION 7

```
310 LDA(ILIM)SUB(INOW)INA(-10)STA(ISHUT)AJP3(950)
    LDA(NS)SUB(NT)AJP(400)AJP3(400)
    LDA(NL)SUB(NLDTI)AJP(410)AJP3(70)
400 CONTINUE
    WRITE OUTPUT TAPE 3,9010
    WRITE OUTPUT TAPE 3,9016,IH
    WRITE OUTPUT TAPE 3,9050,GMAS,TMAS,PNUM
    WRITE OUTPUT TAPE 3,9080,COX,COY
    WRITE OUTPUT TAPE 3,9012,RXI(1),RZI(1),EV,DTI
    WRITE OUTPUT TAPE 3,9090,BX,BZ,EI,IXP,IYP,IZP
    WRITE OUTPUT TAPE 3,9014,EXA,EXB,FXA,CVR,BENERGY
    WRITE OUTPUT TAPE 3,9015,PEXA,PEXB,PFXA
    WRITE OUTPUT TAPE 3,9060,TIME,THERM,CELS,NT
    WRITE OUTPUT TAPE 3,9030
    LDA(NSHUT)AJP1(700)
```

SECTION 8

```
410 DO 500 I=1,LL
500 LDA(ZE)STA1(PPE)STA1(PTE)STA1(PKE)
    LDA(LL)SAU(L+2)ENI1(0)ENI(0)
510 ISK1(*)SLJ(L+2)SLJ(600)ENI(0)
    LDA1(LCUT)AJP1(510)
    LDA(LL)SAU(L+3)
    ENA1(0)SAL(IP1)LIL2(IP1)ENI(0)
520 ISK2(*)SLJ(L+2)SLJ(510)ENI(0)
    LDA2(LCUT)AJP1(520)
540 DRX=RX(J)-RX(I)
    +SSK(DRX),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    DRY=RY(J)-RY(I)
    +SSK(DRY),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    DRZ=RZ(J)-RZ(I)
    +SSK(DRZ),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    LDA(DRX)FMU(DRX)STA(DIST)LDA(DRY)FMU(DRY)FAD(DIST)STA(DIST)LDA(DRZ
   1)FMU(DRZ)FAD(DIST)STA(DIST)FSB(ROE2)AJP2(520)
556 DIST = SQRTF(DIST)
    FNA1(0)INA(-1)AJP1(560)ENI(0)
    POT=PPOTF(DIST)-PPTC
    GO TO 565
560 POT=POTF(DIST)-PTC
565 PPE(I)=PPE(I)+0.5*POT
    PPE(J)=PPE(J)+0.5*POT
    TPOT = TPOT + POT
570 SLJ(520)
600 CONTINUE
```

SECTION 9

```
    ENI1(1)ENI(0)
    I=1
    PKE(1)=HGMAS*(VX(1)*VX(1)+VY(1)*VY(1)+VZ(1)*VZ(1))
    FAD(TPKE),STA(TPKE),LDA1(PKE),FAD1(PPE),STA1(PTE).
    PKEY(1)=HGMAS*(VY(1)*VY(1))
    LDA(LL)SAU(L+2)ENI1(1)ENI(0)
610 ISK1(*)SLJ(L+2)SLJ(660)ENI(0)
    PKE(I)=HTMAS*(VX(I)*VX(I)+VY(I)*VY(I)+VZ(I)*VZ(I))
    FAD(TPKE),STA(TPKE),LDA1(PKE),FAD1(PPE),STA1(PTE).
    PKEY(I)=HTMAS*(VY(I)*VY(I))
    SLJ(610)
```

SECTION 10

```
660 LDA(NS)SUB(NT)AJP(700)AJP2(753)
700 DO 750 I=1,LL
    DX(I)=RX(I)-RXI(I)
    DY(I)=RY(I)-RYI(I)
    DZ(I)=RZ(I)-RZI(I)
    LDA1(PTE),FSB(THERM),AJP3(750).
    WRITE OUTPUT TAPE 3,9020, I,DX(I),DY(I),DZ(I),VX(I),VY(I),VZ(I),
   1PKE(I),PPE(I),PTE(I),PKEY(I)
750 CONTINUE
    TE=TPOT+TPKE
    WRITE OUTPUT TAPE 3,9000
    WRITE OUTPUT TAPE 3,9070,TPKE,TPOT,TE
    WRITE OUTPUT TAPE 3,9093,NPAGE
```


SECTION 11

```
    NPAGE=NPAGE+1
    NS=NS+ND
    LDA(NSHUT)AJP1(950)
753 LDA(NT)SUB(NTT)AJP(950)AJP2(950)
    ISS=1
    LDA(NT)INA(-6)AJP3(765)LDA(TPOT)FSB(QUIT)AJP3(900)
    EMAX=0.0
    DO 760 I=1,LL
    LDA1(PKE)FSB(FM)AJP3(760)LDA1(PPE)FSB(FM)AJP3(757)
    LDA(EMAX)FSB1(PKE)AJP2(760)LDA1(PKE)STA(EMAX)SIL1(ISS)SLJ(760)
757 LCUT(I)=1
760 CONTINUE
765 LDA(ISS)INA(-1)AJP(770)SLJ(780)
770 VOL=SQRTF(PKE(1)/HGMAS)
    GO TO 790
780 VOL=SQRTF(PKE(ISS)/HTMAS)
790 DT=DTI*CVD/VOL
    LDA(DT)FSB(SLOW)AJP2(950)
    NL=
    GO TO 68
```

SECTION 12

```
  900 RAO(NSHUT)SLJ(400)
  950 CONTINUE
      WRITE OUTPUT TAPE 3,9090,BX,BZ,EI,IXP,IYP,IZP
      WRITE OUTPUT TAPE 3,9012,RXI(1),RZI(1),EV,DTI
      WRITE OUTPUT TAPE 3,9091,NT,NS,NPAGE,TIME,DT,DXS,DYS,DZS
      WRITE OUTPUT TAPE 3,9096
      WRITE OUTPUT TAPE 3,9092,(I,RX(I),RY(I),RZ(I),VX(I),VY(I),VZ(I),PK
     1E(I),PPE(I),LCUT(I),I=1,LL)
      WRITE OUTPUT TAPE 3,9093,NPAGE
```

SECTION 13

```
      NPAGE=NPAGE+1
      WRITE OUTPUT TAPE 3,9095
      LDA(LL)SAU(959)ENI1(1)ENI(0)
  955 ENA1(0)INA(-106)AJP2(959)ENI(0)LDA1(VY)AJP3(L+2)SLJ(959)ENI(0)
      LDA1(RY)AJP3(958)LDA1(PKEY)SUB(BENERGY)AJP3(959)ENI(0)
  958 B=1.0/SQRTF(PKE(I)/HTMAS)
      DCOSX=VX(I)*B
      DCOSY=VY(I)*B
      DCOSZ=VZ(I)*B
      WRITE OUTPUT TAPE 3,9094,(I,RX(I),RY(I),RZ(I),DX(I),DY(I),DZ(I),
     1VX(I),VY(I),VZ(I),DCOSX,DCOSY,DCOSZ,PKEY(I),LCUT(I),KCUT(I))
  959 ISK1(*)SLJ(955)
  960 CONTINUE
      WRITE OUTPUT TAPE 3,9093,NPAGE
 1000 LDA(ISHUT)AJP3(9999)
      IF(SENSE SWITCH 2) 9999,4
 9999 STOP
      END
      END
```

B. SPOTA LISTING

SECTION 1

```
      PROGRAM SPOTA
C
C THIS PROGRAM SUBTRACTS THE SURFACE BINDING ENERGY FROM PKEY, RECALCU-
C LATES VY AND DRAWS THE SPOT PATTERN FOR THE (111) ORIENTATION.  THIS
C IS DONE BY PLOTTING THE REPRESENTATIVE AREA, ROTATING THIS ABOUT THE
C Z-AXIS AND PLOTTING, AND ROTATING THE ORIGINAL ABOUT THE X-AXIS AND
C PLOTTING.  NEXT, THE AXES WERE ROTATED +30 DEGREES, THE POINTS WERE
C MIRRORED ABOUT THE X-AXIS AND THEN THE AXES WERE ROTATED -30 DEGREES
C AND A PLOT MADE.  THIS PROCEDURE IS THEN REPEATED WITH A MIRROR ABOUT
C THE ZAXIS INSTEAD OF THE X-AXIS.  THE LAST PLOT RESULTS FROM ROTATING
C THE AXES +60 DEGREES, MIRRORING ABOUT THE NEW Z-AXIS AND ROTATING THE
C AXES -60 DEGREES AND PLOTTING.
C
      DIMENSION VX(1100),VY(1100),VZ(1100),PKEY(1100),ITITLE(12),BENERGY
     1(50),XP(6600),ZP(6600)
      COMMON VX,VY,VZ,PKEY,XP,ZP
 9100 FORMAT(6A8/6A8)
 9200 FORMAT(9E8.2)
 9300 FORMAT(I5,15F5.1)
 9400 FORMAT(I3)
```

SECTION 2

```
      READ 9100,(ITITLE(I),I=1,11)
      READ 9300,KM,(BENERGY(K),K=1,KM)
      READ 9400,ICARDS
      HTMAS=0.332E-6
      LABEL=4H
      TWO=2.0
      BET=0.0
C
C CROT1, CROT2, CROT3, CROT4, CROT5, CROT6 ARE ALL CONSTANTS USED TO
C EFFECT THE NECESSARY ROTATIONS
C
      CROT1=0.5
      CROT2=0.866
      CROT3=CROT1*CROT1
      CROT4=CROT2*CROT2
      CROT5=CROT1*CROT2
      CROT6=CROT4-CROT3
      IPOINTS=ICARDS*3
      READ 9200,(VX(I),VY(I),VZ(I),I=1,IPOINTS)
      LDA(KM)SAU(7016)ENI3(1)ENI(0)
 7000 LDA(IPOINTS)SAU(7002)ENI1(1)ENI2(0)
 7001 LDA1(VY)FMU1(VY)FMU(HTMAS)FSB3(BENERGY)AJP3(7002)AJP(7002)
      INI2(1)FDV(HTMAS)STA2(VY)LDA1(VX)STA2(VX)LDA1(VZ)STA2(VZ)
 7002 ISK1(*)SLJ(7001)ENA2(0)STA(IPOINTS)SAU(7004)ENI2(1)ENI4(0)
```

```
      LPOINTM=IPOINTS*6
      C=0.0
7003  VY(J)=SQRTF(VY(J))
      INI4(1)ENI(0)
      B=VZ(J)/VY(J)
      A=VX(J)/VY(J)
      LDA(A)STA4(XP)LDA(B)STA4(ZP)
      INI4(1)ENI(0)
      LDA(B)STA4(ZP)LAC(A)STA4(XP)
      INI4(1)ENI(0)
      TEMP1=CROT6*A+2.0*B*CROT5
      TEMP2=-CROT6*B+2.0*A*CROT5
      LDA(TEMP2)STA4(ZP)LDA(TEMP1)STA4(XP)
      INI4(1)ENI(0)
      LDA(TEMP2)STA4(ZP)LAC(TEMP1)STA4(XP)
      INI4(1)ENI(0)
      TEMP2=-CROT6*B-2.0*CROT5*A
      TEMP1=CROT6*A-2.0*CROT5*B
      LDA(TEMP1)STA4(XP)LDA(TEMP2)STA4(ZP)
      INI4(1)ENI(0)
      LAC(TEMP1)STA4(XP)LDA(TEMP2)STA4(ZP)
      ENA4(0)STA(LPOINTS)INA(-30)AJP(7500)
      AJP3(7400)ENI(0)
7400  LDA(LPOINTS)SUB(LPOINTM)AJP3(7004)ENI(0)
7410  LDA(C)AJP(7411)AJP3(7411)ENA(0)
      INA(3)STA(MOD)SLJ(7412)ENI(0)
7411  ENA(0)STA(MOD)
      BET=BET+BENERGY(K)
      ITITLE(12)=ICODE(BET)
7412  CALL DRAW(LPOINTS,XP,ZP,MOD,2,LABEL,ITITLE,0.5,0.5,4,4,2,2,8,8,0,L
     1AST)
      SLJ(7004)ENI(0)
7500  LDA(LPOINTS)SUB(LPOINTM)AJP(7410)ENI(0)
      LDA(C)AJP(7510)AJP3(7510)ENI(0)
      ENA(0)INA(2)STA(MOD)SLJ(7511)
7510  ENA(0)INA(1)STA(MOD)ENI(0)
```

```
      BET=BET+BENERGY(K)
      ITITLE(12)=ICODE(BET)
7511  CALL DRAW(30      ,XP,ZP,MOD,2,LABEL,ITITLE,0.5,0.5,4,4,2,2,8,8,0,L
     1AST)
      LPOINTM=LPOINTM-30
      ENI4(0)ENI(0)
      C=1.0
7004  ISK2(*)SLJ(7003)
7016  ISK3(*)SLJ(7000)
      END
```

```
C                                                                       00007750
      FUNCTION ICODE (ANUMBER)                                          00007760
C         CODES ABSOLUTE VALUE OF A FLOATING POINT NUMBER (BETWEEN      00007770
C         1.0E-100 AND 1.0E+100) INTO 8-CHARACTER BCD WORD OF THE FORM  00007780
C         1.23E+45. ICODE = 8H0.00E+00 IF MAGNITUDE OUT OF RANGE.       00007790
*         CHECK AVAILABILITY OF LIBRARY FUNCTIONS IN FORTRAN 62-3.      00007800
      DIMENSION II(8)                                                   00007810
      BNUMBER = ABSF(ANUMBER)                                           00007820
      IF(BNUMBER - 1.0E+100)7,6,6                                       00007830
    7 IF(BNUMBER - 1.0E-100)6,6,2                                       00007840
    6 ICODE = 8H0.00E+00                                                00007850
      RETURN                                                            00007860
C         THIS IS ERROR EXIT.                                           00007870
    2 CALL SCALEIT (BNUMBER, ISCAL10, FACTOR, 3)                        00007880
      ISIGNSC = XSIGNF(1,ISCAL10)                                       00007890
      ISCAL10 = XABSF(ISCAL10)                                          00007900
      IFACT = FACTOR*100.001                                            00007910
      II(8) = XMODF(ISCAL10,10)                                         00007920
      II(7)=ISCAL10/10                                                  00007930
      IF(ISIGNSC)4,3,3                                                  00007940
    3 II(6) = 8H        +                                               00007950
      GO TO 5                                                           00007960
    4 II(6) = 8H        -                                               00007970
    5 II(5) = 8H        E                                               00007980
      II(4) = XMODF(IFACT,10)                                           00007990
      II(3) = (XMODF(IFACT,100))/10                                     00008000
      II(2) = 8H        .                                               00008010
      II(1) = IFACT/100                                                 00008020
      CALL IPACK (II, IPACKED)                                          00008030
      ICODE = IPACKED                                                   00008040
      RETURN                                                            00008050
      END                                                               00008060
C                                                                       00008070
      SUBROUTINE SCALEIT (ANUMBER,ISCAL10,FACTOR,MODE)                  00008080
C         FINDS FACTOR (BETWEEN 1.0 AND 9.99...) AND SCALE OF 10 AS     00008090
C         DEFINED BY     ANUMBER = FACTOR*10.**ISCAL10.                 00008100
C         MODE IS THE NUMBER OF SIGNIFICANT FIGURES REQUIRED. THIS MUST 00008110
C         BE BETWEEN 1 AND 10 OR IT WILL BE PUT EQUAL TO SIX.           00008120
```

```
*          CHECK AVAILABILITY OF LOG10F IN FORTRAN 62-3.                  00008130
      ISCAL10=LOG10F(ANUMBER)                                             00008140
      FACTOR = ANUMBER/10.**ISCAL10                                       00008150
      IF(FACTOR - 0.1)1,2,2                                               00008160
    1 FACTOR = FACTOR*100.                                                00008170
      ISCAL10 = ISCAL10 - 2                                               00008180
      GO TO 8                                                             00008190
    2 IF(FACTOR - 1.0)3,8,4                                               00008200
    3 FACTOR = FACTOR*10.                                                 00008210
      ISCAL10 = ISCAL10 - 1                                               00008220
      GO TO 8                                                             00008230
    4 IF(FACTOR - 100.0)6,5,5                                             00008240
    5 FACTOR = FACTOR/100.                                                00008250
      ISCAL10 = ISCAL10 + 2                                               00008260
      GO TO 8                                                             00008270
    6 IF(FACTOR - 10.0)8,7,7                                              00008280
    7 FACTOR = FACTOR/10.                                                 00008290
      ISCAL10 = ISCAL10 + 1                                               00008300
    8 IF(MODE)9,9,10                                                      00008310
    9 MODE = 6                                                            00008320
      GO TO 11                                                            00008330
   10 IF(MODE - 10)11,11,9                                                00008340
   11 IFACTOR = FACTOR*10.**(MODE - 1) + 0.5                              00008350
      FACTOR = IFACTOR                                                    00008360
      FACTOR = FACTOR/10.**(MODE - 1)                                     00008370
      IF(FACTOR - 10.)13,12,12                                            00008380
   12 FACTOR = 1.                                                         00008390
      ISCAL10 = ISCAL10 + 1                                               00008400
   13 RETURN                                                              00008410
      END                                                                 00008420
C                                                                         00008430
      SUBROUTINE IPACK (II, IPACKED)                                      00008440
C         TAKES 8 SIX-BIT WORDS AND PACKS THEM LEFT TO RIGHT              00008450
C         IN IPACKED. IF WORD IS ZERO, 12B IS SUBSTITUTED.                00008460
*         CONVERT TO CODAP FOR FORTRAN 62-3.                              00008470
      CON(IZERO = 12B).                                                   00008480
       SIU1(ISAVE)      ENI1(8).                                          00008490
 1NEX  LDA1(II)         AJP1(2NEX).                                       00008500
       LDA (IZERO).                                                       00008510
 2NEX  LRS (6)          INI1(-2).                                         00008520
       ISK1(-1)         SLJ (1NEX).                                       00008530
       STQ (IPACKED)    LIU1(ISAVE).                                      00008540
      END                                                                 00008550
      END
```

APPENDIX II

A. Program TWOPOT

Section designations correspond to those of part A of Appendix I.

Section 1: The form of the potential (Born-Mayer) is established for both types of interactions. Necessary space is reserved in the computer memory for all quantities. Input and output formats are established.

Section 2: Various quantities used throughout the program are established and input data is read.

Section 3: The microcrystallite is constructed and any desired surface irregularity is introduced.

Section 4: Initial velocity of the primary is established in accordance with the input data and crystallite construction is completed.

Section 5: The force calculation technique is applied and all atoms relocated accordingly. New velocities of all atoms are calculated.

Section 6: The positions of all atoms are tested against the original crystal boundaries and the atoms are indexed accordingly.

Section 7: If output is called for at this point, headings are printed.

Section 8: All required separation distances are calculated and the potential energy of each atom is found.

Section 9: Kinetic energy is calculated for all atoms.

Section 10: Output is printed when the proper time step is reached. All atoms with a total energy in excess of 0.25 eV are included.

Section 11: All atoms with potential energy less than 1.0 $\times 10^{-10}$ eV are indexed and excluded from here on from force calculations. The time step interval is recalculated based on the most energetic atom still in the crystal. The run is terminated if the total potential energy has dropped to less than 0.5 eV or if a designated number of time steps have been completed. Otherwise, the run is recycled for another time step.

Section 12: The end-of-run summary of positions, velocities, and energies is printed if called for.

Section 13: The velocity, position, and kinetic energy of all atoms are tested and a summary printed for all atoms with negative y-velocity and negative y-position. Included also are those atoms with positive y-position, negative y-velocity, and kinetic energy greater than 2.0 eV. Program is returned to the data input point for insertion of a new set of data.

B. Program SPOTA

Section designations correspond to those of part B of Appendix I.

Section 1: Necessary space is reserved in the computer memory for all quantities. Input and output formats are established.

Section 2: Various quantities used throughout the program are established and input data is read.

Section 3: Kinetic energy in the direction perpendicular to the bombarded surface is tested against a value of binding energy. If the kinetic energy is greater,

the binding energy is subtracted and a new perpendicular velocity found. If it is less, the atom is excluded from further calculations.

Section 4: The ratios VX/VY and VZ/VY are found and plotted respectively on the horizontal and vertical axes of a graph. The program is recycled for a new value of binding energy.

Section 5: FUNCTION ICODE, SUBROUTINE SCALEIT, and SUBROUTINE IPACK are extracted from the DRAW routine to enable the variable binding energy to be recorded on each graph.

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13. ABSTRACT

Sputtering of monocrystalline copper, a face-centered cubic, was investigated by computer simulation techniques using the Born-Mayer potential. Normally incident argon ions were shot into the (111), (110), and (100) orientation at various energies. Qualitatively correct deposit patterns were obtained for all orientations. Surface irregularities were found to play a significant role in the sputtering mechanism. Approximate values for the surface binding energy on the (111) and (110) orientations were 2.25 eV and 2.0 eV, respectively.

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